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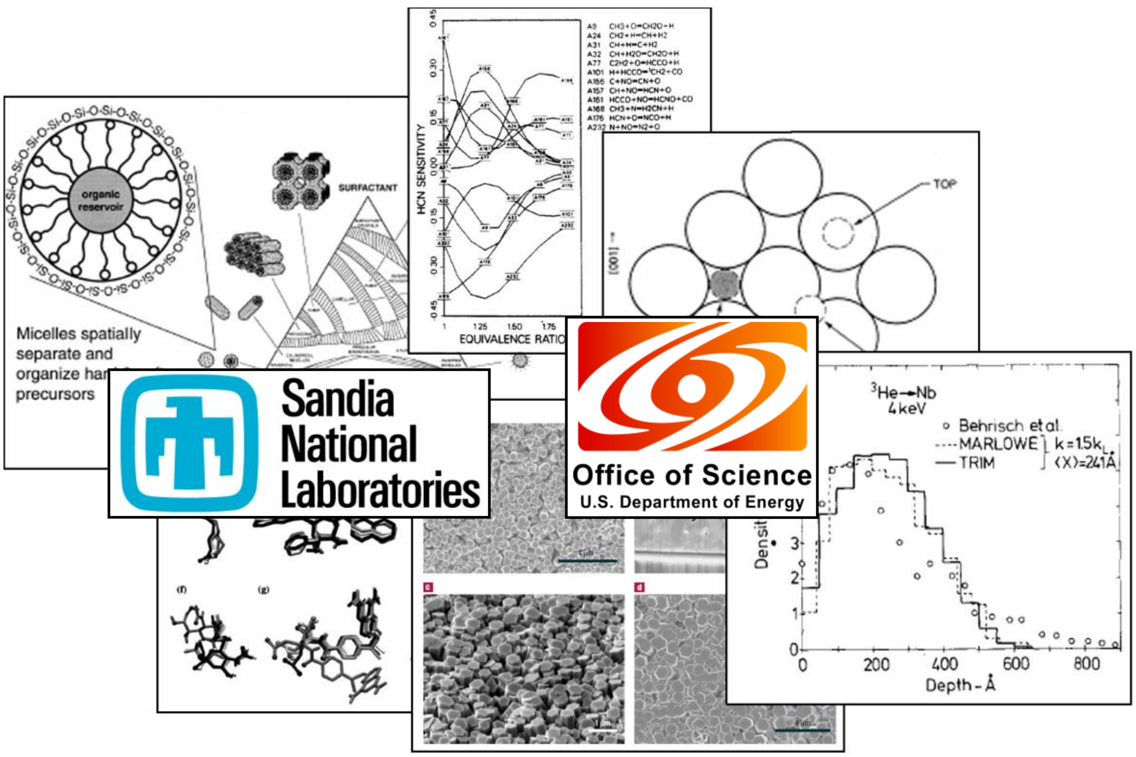
A Brief History of Sandia National Laboratories and the Department of Energy's Office of Science:

Interplay between Science, Technology, and Mission



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A Brief History of Sandia National Laboratories and the Department of Energy's Office of Science: Interplay between Science, Technology, and Mission

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Abstract

In 1957, Sandia National Laboratories (Sandia) initiated its first programs in fundamental science,[a] in support of its primary nuclear weapons mission. In 1974, Sandia initiated programs in fundamental science supported by the Department of Energy's Office of Science (DOE-SC). These latter programs have grown to the point where, today in 2011, support of Sandia's programs in fundamental science is dominated by that Office.

In comparison with Sandia's programs in technology and mission applications, however, Sandia's programs in fundamental science are small. Hence, Sandia's fundamental science has been strongly influenced by close interactions with technology and mission applications. In many instances, these interactions have been of great mutual benefit, with synergies akin to a positive "Casimir's spiral"[b] of progress.

In this report, we review the history of Sandia's fundamental science programs supported by the Office of Science. We present: (a) a technical and budgetary snapshot of Sandia's current programs supported by the various suboffices within DOE-SC; (b) statistics of highly-cited articles supported by DOE-SC; (c) four case studies (ion-solid interactions, combustion science, compound semiconductors, advanced computing) with an emphasis on mutually beneficial interactions between science, technology, and mission; and (d) appendices with key memos and reminiscences related to fundamental science at Sandia.

[a] At the time, Sandia's fundamental science programs were dominated by the physical and chemical sciences.

[b] As discussed in Section 1 of this report, we refer to a Casimir's Spiral as a mutually beneficial interaction between science and technology in which: science enables new tools and technology, and these tools and technology likewise enable new science.

Acknowledgements

We gratefully acknowledge contributions and edits from: Charles Barbour, Will Bolton, Jeff Brinker, Mike Coltrin, Laurence S. Costin, Randy Cygan, Doris Desimone, Barney Doyle, Grant Heffelfinger, Mark Ivey, Quinn Johnson, Gary Kellogg, Jennifer Lange, Len Lorence, Kevin McCarty, David R. Myers, James E. Martin, Rich Nygren, Robin Reeves, and Bill Wampler. We especially acknowledge extremely thorough comments from Alyssa Christy and Blythe Clark.

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Cover Figure

A collage of figures from various highly cited papers written at Sandia National Laboratories and supported by the Office of Science. Left-Right, Top-Bottom:

1. Brinker, CJ, YF Lu, A Sellinger and HY Fan (1999). "Evaporation-Induced Self-Assembly: Nanostructures Made Easy." Advanced Materials **11**(7): 579-+. [776] : [<DOE-SC><NSF/NIH><LDRD>]
2. Miller, JA and CT Bowman (1989). "Mechanism and Modeling of Nitrogen Chemistry in Combustion." Progress in Energy and Combustion Science **15**(4): 287-338. [1477] : [<DOE-SC>]
3. Daw, MS and MI Baskes (1984). "Embedded-Atom Method - Derivation and Application to Impurities, Surfaces, and Other Defects in Metals." Physical Review B **29**(12): 6443-6453. [2783] : [<DOE-SC>]
4. Morris, GM, DS Goodsell, RS Halliday, R Huey, WE Hart, RK Belew and AJ Olson (1998). "Automated Docking Using a Lamarckian Genetic Algorithm and an Empirical Binding Free Energy Function." Journal of Computational Chemistry **19**(14): 1639-1662. [2720] : [<DOE-SC><NSF/NIH>]
5. Tian, ZRR, JA Voigt, J Liu, B McKenzie, MJ McDermott, MA Rodriguez, H Konishi and HF Xu (2003). "Complex and Oriented Zno Nanostructures." Nature Materials **2**(12): 821-826. [499] : [<DOE-SC><LDRD>]
6. Biersack, JP and LG Haggmark (1980). "A Monte-Carlo Computer-Program for the Transport of Energetic Ions in Amorphous Targets." Nuclear Instruments & Methods **174**(1-2): 257-269. [3520] : [<DOE-SC>]

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1 Introduction

Sandia National Laboratories' history began in 1949 when Sandia, as a division of Los Alamos Scientific Laboratory, was asked to take responsibility for the non-nuclear (ordnance) pieces of our nation's nuclear weapons. These pieces have now come to include:

- Research, design and development of non-nuclear components: Sandia is responsible for the design and development of 96 percent of the approximately 6,300 components of a modern nuclear weapon system (see, e.g., Figure 1), including a complex array of mechanical and electrical systems and software for the control, navigation, safety and security of nuclear warheads.
- Life extension of nuclear weapons.
- Manufacturing of neutron generators, custom microelectronics and microsystems, and development of other custom components for manufacture by others.
- Support for the Stockpile including maintenance, surveillance, logistics, dismantlement, and acting as a military liaison: Sandia is responsible for ancillary equipment used worldwide by the U.S. military to control, handle, ship, store, and maintain nuclear weapons.
- Nuclear materials protection.

These non-nuclear pieces are fundamentally tied to a wide gamut of materials and natural phenomena. Hence, in order to ensure their safety, security and reliability, Sandia has long had an interest in developing a scientific understanding of the diverse materials and natural phenomena relevant to nuclear weapons at the deepest possible level. This interest was further nurtured by AT&T Bell Laboratories, which managed Sandia for many years and set the tone at Sandia for a culture of outstanding science and outstanding scientists.[3]

By 1957, Sandia had formulated plans for a fundamental research program in physics and physical chemistry, with emphases on solid-state physics, radiation effects, combustion processes, physical electronics, hydro-magnetics, high-temperature physics, theoretical mechanics and geophysics.[4] By

Figure 1: B83 bomb with some of its 6,300 parts.

1958, work on the first two of these had been initiated.[5] For example, new staff were being hired in radiation effects with the goal of achieving new and fundamental understanding, and a large new tool (a 2 MeV van de Graaff generator) had been ordered for the purpose of tailored irradiation of solids with particles of known type and energy.

Thus, as illustrated schematically in Figure 2(a), Sandia gradually developed efforts in science, as well as in tools and technologies, that were considered well connected to its nuclear weapons mission. Importantly, these efforts interacted significantly with each other, while taking place simultaneously within a single (albeit large) organization.

In this article, we give a brief history of Sandia's most fundamental solid-state, chemical, and mathematical science programs – those that came to be supported by the Department of Energy's Office of Science (DOE-SC). Our primary purpose is to use this history as an opportunity to explore those instances in which there have been strong positive interactions between science, technology and mission.[6] Along the way, we highlight some of Sandia's highest impact science supported by DOE-SC. However, these examples are not covered in depth: the story of Sandia's highest impact science supported by DOE-SC, independent of its

[3] Among a long string of Presidents of Sandia drawn from AT&TBell Labs were: Julius Molnar, John Hornbeck, Morgan Sparks, and George Dacey. Among a long string of Vice Presidents of Research at Sandia drawn from AT&T Bell Labs were: RC Fletcher, John K. Galt, Bill Brinkman, Venky Naryanamurti, and Paul Fleury.

[4] RS Claassen, "Presentation to MJ Kelley on Fundamental Research at Sandia" (1957), included as Appendix 1 of this report.

[5] FL Vook, "Frederick L. Vook and Sandia Solid State Science 1958-1994" (2006), included as Appendix 2 of this report.

[6] Throughout this article, we distinguish between science, technology, and mission application. As recently discussed [JY Tsao, WB Gauster, KW Boyack, ME Coltrin, JG Turnley, Galileo's Stream: A Framework for Technical Knowledge Production, Research Policy **37**, 330-352 (March, 2008)], these three categories of knowledge can be thought of more generally as "science and understanding," "tools and technology," and "societal use and behavior." Together they form an interacting and mutually reinforcing triangle of knowledge.

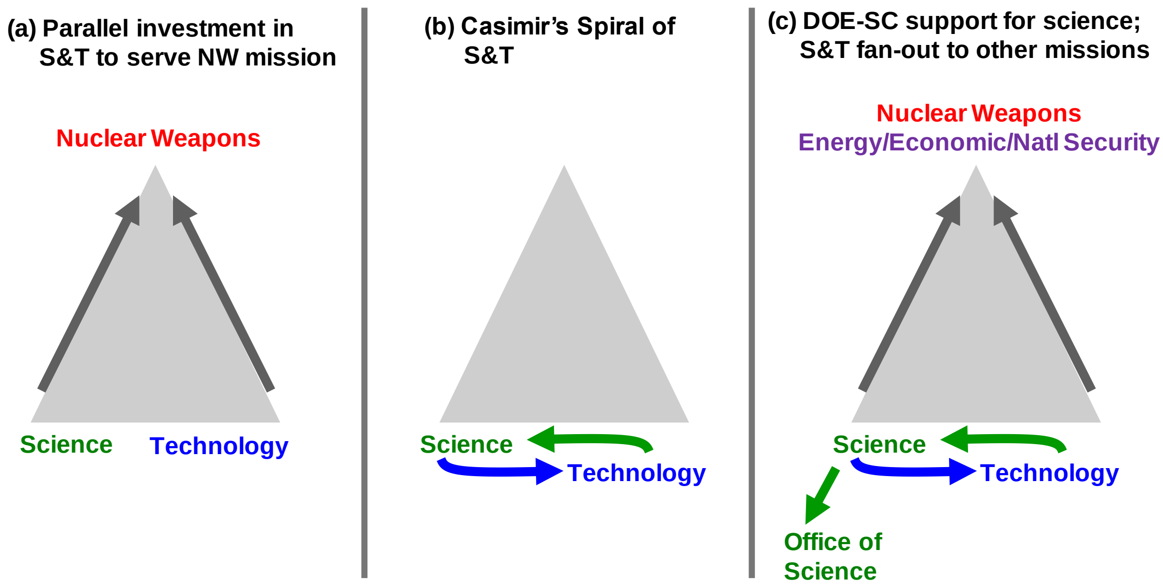


Figure 2: Historical progression of interactions between science, technology and mission at Sandia. Science, technology and mission are depicted as the vertices of a triangle, with the directed edges representing contributions made by one to another. (a) The origins of Sandia's science and technology (S & T) investments were motivated by the contributions they could make to Sandia's nuclear weapons mission. (b) The subsequent interaction between science and technology "under one roof" led in some cases to a Casimir's Spiral of positive contributions that science and technology made to each other. (c) Some of Sandia's science came to be supported by the Department of Energy's Office of Science, distinct from that supported by Sandia's mission areas. At the same time, Sandia's mission expanded to include energy, as well as economic and national security.

interactions with technology and mission, is interesting, important, and deserving of its own separate document.

Our emphasis throughout is on those instances for which interactions with technology and mission are strongly positive, though we are well aware that these interactions can actually be both negative and positive.

Consider first the influence of technology on science. On the one hand, a desire to be relevant to a technology could narrow the research choices a scientist might otherwise make, and could be expected to reduce, on average, the quality of the science.[7] On the other hand, modern science depends increasingly on tools with a high technology content.[8] Close access to technology could thereby add a new dimension to the science that is done, and might be expected to improve the quality of the science.

Consider second the influence of science on technology. On the one hand, developing a greater scientific understanding of a technology requires resources that might otherwise have been spent on promising empirical avenues for improving the technology, and hence could slow its progress.[9] On the other hand, a greater scientific understanding of a technology might open up otherwise unimagined technology possibilities. Exposure to science can add a new dimension to technology, and hence enhance its progress (as with, e.g., the Manhattan Project).

In the ideal case, the influences in both directions are positive and so powerful that they fuel a "Casimir's Spiral" like that illustrated in Figure 2(b) in which science enables new tools and technology, and these tools and technology likewise enable new science.[10,11] AT&T Bell Laboratories at its zenith[12] is the quintessential example of an environment in which the net sum of the influences is widely believed to be hugely positive. Having been managed for much of its history by AT&T, and having drawn many of its research vice-presidents from AT&T Bell

[7] RK Merton, The Sociology of Science: Theoretical and Empirical Investigations (The University of Chicago Press, 1973).

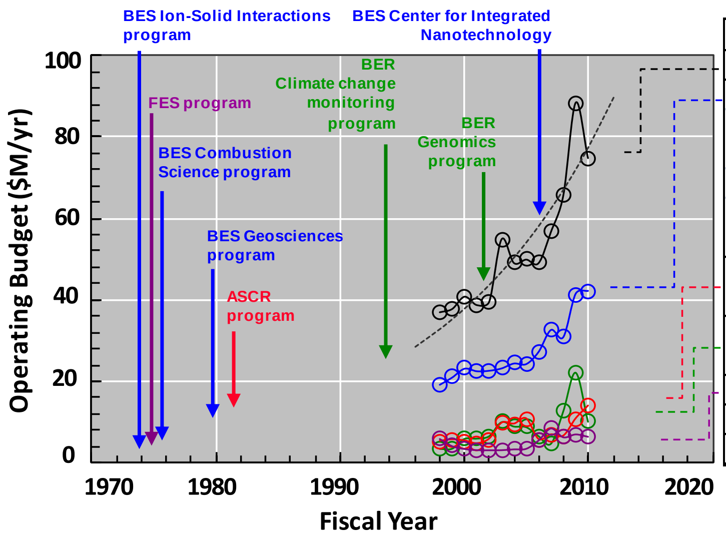
[8] H Brooks, The relationship between science and technology, Research Policy 23, 477-486 (1994).

[9] N Rosenberg, Inside the Black Box: Technology and Economics (Cambridge University Press, 1982); H. Petroski, Engineering ≠ Science, IEEE Spectrum (December, 2010), p. 8.

[10] HBG Casimir, Haphazard Reality -- Half a Century of Science (Harper & Row, 1983).

[11] J Mokyr, The Gifts of Athena: Historical Origins of the Knowledge Economy (Princeton University Press, 2002).

[12] S Millman, Ed., A History of Engineering and Science in the Bell System: Physical Sciences 1925-1980 (AT&T Bell Laboratories, 1983).



Program Area and FY10 Operating Budget ($M/yr)		
All		74.9
Basic Energy Sciences	BES	42.1
Materials Science & Engineering	MSE	14.0
Scientific User Facilities	SUF	11.3
Chemical Sciences, Geosciences & Biosciences	CSGB	16.8
Advanced Scientific Computing Research	ASCR	13.9
Biological and Environmental Research	BER	10.1
Fusion Energy Sciences	FES	6.4
Nuclear Physics	NP	0.0
Miscellaneous		2.4

Figure 3: Twelve-year operating budget history of Sandia's Office of Science programs within the context of >35 years of fundamental science programs (left), and snapshot of the fiscal year 2010 operating budget, organized by sponsoring Office of Science sub-office or division (right). Note that the graph plots both budget provided to Sandia directly from the Office of Science as well as budgets provided indirectly to Sandia from the Office of Science via other institutions. Also, note that the graph plots only operating, not capital, budget. Over the years, the operating budget has been roughly 85.7%, and the capital budget 14.3%, of the total budget.

Laboratories during those years (1949-1993), [13] Sandia might be a similar example.

In a less ideal case, however, the net sum of the influences might be negative, in which case there is no integrated benefit to the organization or to the nation from having the two activities "under one roof."

Thus, in emphasizing those instances for which interactions with technology and mission are strongly positive, we understand that we are leaving out those instances in which they might have been negative. Our intent therefore is not to make the quantitative claim that Sandia is indeed an example for which the net sum of the influences is hugely positive. We instead wish to make a qualitative case to illustrate a wide variety of individual examples for which the influences are positive.

Finally, although Sandia's nuclear weapons mission was its earliest and still its most important, Sandia's mission has broadened and come to include the entire space of missions and societal uses quoted in the mission statement of the Department of Energy's Office of Science: energy, economic and national security. In this report, we include these other missions in our discussions of the interactions between science, technology and mission.

[13] L Johnson, Sandia National Laboratories: A History of Exceptional Service in the National Interest, Sandia Report 97-1029 (Sandia National Laboratories, 1997).

2 Overview of Office of Science Programs at Sandia

As discussed in the previous section, fundamental science at Sandia dates back to 1958. By 1974, that science had developed to the point of attracting the attention of the Atomic Energy Commission's Division of Physical Research (which later became folded into the Energy Research and Development Administration and ultimately the current Department of Energy Office of Science), and a program at Sandia supported by that Office was initiated in the area of ion-solid interactions.

Although in the early years (1970's and 1980's) this source of support for science was small compared to that from Sandia's nuclear weapons mission, in more recent years (1990's and 2000's) it has come to be Sandia's dominant source of support for fundamental science. By FY2010, Office of Science support represented \$75M in operating budget, an average growth rate of \$75M/36yrs = 2.1\$M/yr.

That growth is illustrated in the twelve-year history of operating budgets for Sandia's Office of Science programs shown in the graph on the left side of Figure 3. The various sub-offices within the Office of Science have gone through many reorganizations over the years, so the graph is organized around the current sub-offices (from which Sandia has derived some support for research): Basic Energy Sciences (BES), Advanced Scientific Computing Research (ASCR), Biological and Environmental Research (BER), Fusion Energy Sciences (FES), and Nuclear Physics (NP).

2.1 Office of Basic Energy Sciences (BES)

Sandia's largest Office of Science program area is supported through the Office of Basic Energy Sciences. This sub-office within the Office of Science is one of the largest sponsors of research in the physical sciences in the world. It funds research at more than 160 research institutions across the nation, and supports: (a) "fundamental research in focused areas of the natural sciences in order to expand the scientific foundations for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy use," as well as (b) "work that creates knowledge and develops tools to strengthen national security." [14] Within Basic Energy Sciences, Sandia has programs in all three of its major divisions: Materials Science and Engineering (MSE); Scientific User Facilities (SUF); and Chemical Sciences, Geosciences and Biosciences (CSGB).

Materials Science and Engineering Division

Within the Materials Science and Engineering Division, Sandia's programs trace their lineage back to Sandia's first Office of Science program in ion-solid interactions, which began in 1974. Since then, they have expanded considerably and now include the following activities:

- Quantum Electronic Phenomena and Structures, focused on fabricating and characterizing low-dimensional semiconductor nanostructures;
- Active Assembly of Dynamic and Adaptable Materials, focused on using living systems to develop materials with programmable transport and adaptive response capabilities;
- Mechanics of Small Length Scales, focused on the role of grain boundaries and defects in determining the structure and properties of metals;
- Novel Electronic Materials, focused on the growth, optical and electronic properties of wide-bandgap AlGaInN alloys;
- Molecular Nanocomposites, focused on the assembly and properties of functional organic-inorganic materials on multiple length scales;
- Field-Structured Composites, focused on novel microstructure formation in self-assembled complex composite materials under time-varying multi-axial magnetic and electric fields; and
- Nanometer-Scale Surface and Interface Phenomena, focused on obtaining the fundamental, nanometer-scale information needed to understand, predict and control the surface and interface properties of materials.
- Light Matter Interactions, focused on understanding energy transfer via control of photonic density of states in order to predict and control light emission and discover new phenomena.

Most recently, in 2009, Sandia was awarded an Energy Frontier Research Center (EFRC) for Solid-State Lighting Science, [15] one of 46 EFRCs nationwide devoted to establishing the scientific foundation for a fundamentally new U.S. energy economy. Sandia's EFRC focuses on the scientific foundation underlying solid-state lighting, an emerging technology that promises very high efficiencies for producing light for general illumination purposes.

Scientific User Facilities Division

Within the Scientific User Facilities Division, Sandia jointly operates, with Los Alamos National Laboratory, a major facility, the Center for Integrated Nanotechnologies (CINT). This facility opened its doors in 2006, with an overarching theme of nanoscience integration: establishing the scientific principles that govern the design, performance and integration of nanoscale materials. The facility is one of BES's five Nanoscale Science Research Centers, and is jointly managed and staffed by Sandia National Laboratories and Los Alamos National Laboratory. Consistent with its theme of nanoscience integration, CINT has three overarching thrusts:

- innovative instrumentation for probing and manipulating nanostructures;
- theory and simulation for modeling; and
- "discovery platforms" (microfabricated platforms for measuring electronic, fluidic, and mechanical properties at the nanoscale).

Chemical Sciences, Geosciences, and Biosciences Division

Within the Chemical Sciences, Geosciences, and Biosciences Division, Sandia's programs were initiated in 1976 with the development and birth of the Combustion Research Facility (CRF) at Sandia's Livermore, California location, and with the initiation around 1980 of smaller activities in geosciences

[14] Office of Basic Energy Sciences(BES) website (http://science.energy.gov/bes/) (accessed Dec, 2010).

[15] Solid-State Lighting Science Energy Frontier Research Center website (http://ssls.sandia.gov/).

involving continental scientific drilling to understand the complex processes of magmatic and hydrothermal systems. [16] At this point, Sandia's programs supported by this Division are larger than those supported by any other Division.

In the area of chemical sciences, the CRF is currently home to about 100 scientists, engineers and technologists, many of whom are supported through the CSGB division. The major CRF program areas supported by CSGB are:

- Combustion Chemistry, focused on understanding the key chemical processes that underlie the complex mechanisms of combustion;
- Reacting Flows, focused on revealing and understanding the interactions between fluid dynamics and combustion chemistry that affect the performance and emissions of combustion devices; and
- Computational Modeling and Simulation, focused on using theory, modeling and simulation tools to better understand problems ranging from fundamental chemical dynamics to the full characterization of the operation of combustion devices.

In the area of geosciences, Sandia's current research focus is on the complex chemical, mechanical, and rheological properties of earth's near-surface materials. Fundamental geoscience projects at Sandia currently funded by the CSGB division include:

- Molecular simulations and spectroscopy of geochemical interfaces to determine molecular structure and dynamical behavior of water and solutes at the surfaces of oxides, hydroxides, and clay minerals;
- Experimental and theoretical analyses of pore scale processes in mudstones, shales, and clays with a focus on groundwater flow, geomechanics, and imaging; and
- Multiphysics and multiscale analysis of the isolation of carbon dioxide and other contaminants in geological reservoirs as part of an Energy Frontier Research Center in partnership with the University of Texas.

2.2 Office of Advanced Scientific Computing Research (ASCR)

Sandia's second largest Office of Science program area is supported through the Office of Advanced Scientific Computing Research (ASCR). This program area's focus is "DOE's world leadership in scientific computation by supporting research in applied mathematics, computer science and high-performance networks and providing the high-performance computational and networking resources that are required for world leadership in science."[17] This program area, begun in the early 1980's, has grown to span a wide range of activities, including:

- Applied Mathematics, particularly methods for translating models of the physical world into software algorithms;
- Computer Science, focused on system software and tools for maximizing the capabilities of high-performance computers; and
- Scientific Discovery through Advanced Computing, focused on coordinated research efforts directed at applying emerging capabilities in terascale and petascale computing to research problems that are insoluble by traditional theoretical and experimental approaches.

2.3 Office of Biological and Environmental Research (BER)

Sandia's next-largest Office of Science program area is supported through the Office of Biological and Environmental Research (BER). This program area supports "environmental and biomedical knowledge that promotes national security through improved energy production, development, and use, international scientific leadership that underpins our Nation's technological advances, and research that improves the quality of life for all Americans."[18] Sandia's involvement in this program area spans four major topics within its two major divisions: Climate and Environmental Sciences; and Biological Systems Science.

Climate and Environmental Sciences Division

A first topic in the Climate and Environmental Sciences division is in helping understand and quantify global climate change through atmospheric radiation measurements (ARM[19]) and atmospheric

[16] CR Carrigan and JC Eichelberger, "Zoning of magmas by viscosity in volcanic conduits," Nature **343**, 248-51 (1990); JC Eichelberger, W Hildreth, and JJ Papike, "The Katmai scientific drilling project, surface phase: Investigation of an exceptional igneous system," Geophysical Research Letters **18**, 1513-16 (1991).

[17] Office of Advanced Scientific Computing Research (ASCR) website (http://science.energy.gov/ascr/).

[18] Office of Biological & Environmental Research website (http://science.energy.gov/ber/).

[19] ARM Climate Research Facility website (http://www.arm.gov).

systems research (ASR). The dates at which key Sandia involvements in this topic began are:

- 1992. Sandia was selected to manage and operate the new Unmanned Aerospace Vehicle (ARM-UAV) Program, aimed at collecting remote sensing and *in situ* data on the interaction between clouds and solar and thermal energy in the troposphere. All together, 13 major flight campaigns were conducted in the continental US, Alaska, Hawaii, and Australia before the ARM-UAV program came to an end in 2006, with continuing aircraft-based measurements folded into the "ARM Aerial Vehicle Program" (ARM-AVP).
- 1993. A Sandia-led team developed the ground-based instrumentation systems that were installed and continue to operate at the three fixed ARM sites in the Tropical Western Pacific (Darwin, Nauru, and New Guinea). Sandia supports DOE-SC/BER and ARM activities world-wide including new deployments, Intensive Operating Periods and field campaigns, and programmatic functions such as advisory reviews.
- 1997. Sandia established the ARM Climate Research Facilities on the North Slope of Alaska in 1997 and has managed those sites since that time.

These atmospheric radiation measurement facilities, along with other fixed and mobile sites in the DOE ARM Program, have made significant contributions to improving climate prediction models through better understanding of radiative heat transfer, radiation absorption, and cirrus cloud properties. The facilities are open platforms through which users worldwide propose and conduct research that target specific science questions, as well as test and validate new instruments. The data gathered from the facilities are also open to atmospheric scientists worldwide for developing and validating climate change models.

A second topic in the Climate and Environmental Sciences division, one that began in 1996, is in helping understand and quantify phenomena related to currently intractable environmental remediation problems, including the geochemistry of the migration of contaminants associated with nuclear waste, and their stabilization in heterogeneous and fractured media.

Biological Systems Science

A first topic in the Biological Systems Science Division, one that began in 2002, is the Genomic Science (formerly the Genomics:GTL or Genomes to Life) program.[20] In one area of this program, Sandia is helping to understand and potentially improve pathways and organisms important for bioremediation of metals and radionuclides. In another area of this program, Sandia is participating in the Joint BioEnergy Institute (JBEI). This Institute began in 2008 and is composed of a group of national laboratories and universities working to advance the development of the next generation of biofuels—liquid fuels derived from the solar energy stored in plant biomass. Among Sandia's contributions to this institute are the development of new processes and technologies to efficiently liberate monomeric sugars from a wide range of biomass feedstocks, a key step in the extraction of useful energy from those feedstocks. Other contributions include the examination of the photosynthetic properties of various plants and microbes, and analysis of extremophile enzymes.

A second topic in the Biological Systems Science Division, the artificial retina project,[21] began in 2003. In this project, Sandia is part of a large group of national laboratories, universities and companies working to develop dramatically improved retinal prosthetics to restore sight to the blind. Sandia's major role is to help develop biocompatible microelectronic circuitry with high-density electrode arrays for communicating with retinal cells. The use of MEMS fabrication techniques enables novel geometries in which connections can be made from both sides of the circuit.

2.4 Office of Fusion Energy Sciences (FES)

A final Sandia Office of Science program area is supported through the Office of Fusion Energy Sciences (FES). This program area, begun in 1975, supports "basic research efforts to advance plasma science, fusion science, and fusion technology - the knowledge base needed for an economically and environmentally attractive fusion energy source."[22] Sandia's current work in this program area involves providing the basic plasma and materials science understanding of plasma-wall interactions.

[20] Office of Biological and Environmental Research Genomics Science Program website (http://genomicscience.energy.gov/program/index.shtml#page=news).

[21] Office of Biological and Environmental Research Artificial Retina Project website (http://artificialretina.energy.gov/about.shtml).

[22] Office of Fusion Energy Sciences website (http://science.energy.gov/fes/).

3 Citation Analysis

At this point in time, Sandia has a 36-year history of support from, and participation in, Office of Science programs. Through that support, Sandia has made significant contributions to science, as documented in many articles published in the open scientific literature, including the highly cited ones listed in Appendix 4.

3.1 Statistics

A subset of these contributions is illustrated at the top of Figure 4, which shows a scatter plot of all of Sandia's journal articles published between 1974 and December 2010, with ≥100 cumulative citations, and contained in the comprehensive web-of-science database of the Institute of Scientific Information.

Each article is represented by a solid white data point and is plotted according to the number of citations it has received through December 2010 and its publication date. To emphasize those articles that have been cited rather heavily, the logarithmic vertical axis spans the two orders of magnitude from 100 to 10,000, and so we plot only those articles that had been cited 100 times or more as of December 2010. These "Century Club" articles represent a very select subset of 838 out of Sandia's total of 29,910 articles. Of these Century Club articles, we have outlined in blue circles those that were supported at least in part by the Office of Science. These articles account for 349, or 42%, of the Century Club articles.

To see how the various sources of support for the Century Club articles have evolved over time, the bottom of Figure 4 shows a scatter plot of the number of articles associated with various sources of support published in a given year. The sources of support were deduced from formal acknowledgments within the articles, as well as, in the absence of such formal acknowledgements, informal queries to authors and program managers. The quantitative results should be considered approximate, however: formal acknowledgements are sometimes incomplete, and informal responses to queries rely on authors' and program managers' memories which can be clouded by time. In cases of articles with multiple sources of support, the articles were treated as fractionally (and equally) supported by each source, so the sum over all sources of support is the same as the number of Century Club articles published that year.

As one can see, DOE-NW/NA (DOE funded articles containing either a nuclear weapons, or no further, attribution within DOE) have historically been the dominant source of highly cited articles. In the early years (1970's and 1980's) this source of support was dominated by the research foundations piece of Sandia's nuclear weapons program.

As this source of support decreased over time, the Office of Science became, beginning in the 1980's, an increasingly important source of highly cited articles. In addition, after Sandia's Laboratory Directed Research and Development (LDRD) program began around 1992, it too became an increasingly important source of highly cited articles.

Note that towards the right of the plot (for the more recent years) the number of highly cited articles appears to decrease. This decrease is not due to a real decrease in scientific productivity, but due to the fact that most articles accumulate citations over a number of years, and the most recent articles have accumulated only a small fraction of the citations they will eventually accumulate.

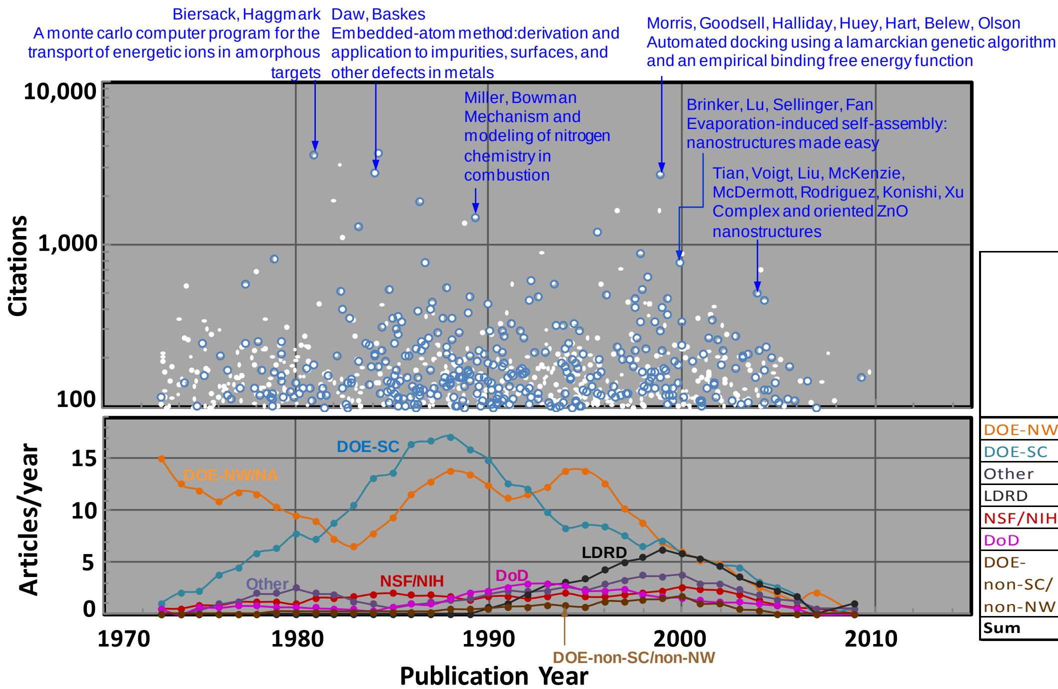
Finally, the table at the right of Figure 4 indicates the fractional importance of the various sources of support over all articles in the Century Club irrespective of year published. The Office of Science accounts for 325, or 39%, of the articles. These are smaller numbers than the 349, or 42%, mentioned above, because here we have accounted for fractional support by multiple sources.

3.2 Highlights

All of the articles plotted in Figure 4, cited 100 times or more, have had exceptional impact on science. To give a flavor for this impact, we discuss briefly, in chronological order, six representative Office-of-Science-supported articles that are very highly cited relative to their peers in the same publication year (data points with arrows indicating their authors and titles).

Note that three (TRIM, EAM, and AutoDock) out of these six articles describe tools or methods for solving scientific problems while themselves making use of deep scientific understanding; they are thus powerful examples of the science-to-technology-to-science "Casimir's Spiral" mentioned earlier. Another two (EISA, and ZnO nanostructures) of these articles describe tools or methods for fabricating materials structures of scientific interest, and are thus examples of technology-to-science synergy. The remaining article (nitrogen chemistry) describes the scientific result (a detailed understanding of nitrogen combustion chemistry) of the use of a wide array of tools developed to study these chemistries, and is thus also an example of technology-to-science synergy.

TRansport of Ions in Matter (TRIM). The first article was by Jochim Biersack (Hahn-Meitner



Funding Source	Cumulative Number	Cumulative Fraction
DOE-NW/NA	325	0.39
DOE-SC	276	0.33
Other	65	0.08
LDRD	61	0.07
NSF/NIH	53	0.06
DoD	43	0.05
DOE-non-SC/non-NW	16	0.02
Sum	**838**	**1.00**

Figure 4: (Top left) Scatter plot of all of Sandia's journal articles published between January 1970 and December 2010 contained in the Institute of Scientific Information web-of-science database, and which had accumulated 100 or more citations through December 2010. (Bottom left) Five-year-running average of articles per year supported by various funding sources. DOE-NW/NA = DOE with either Nuclear Weapons or no further attribution within DOE; DOE-SC = DOE Office of Science; LDRD = Sandia's Laboratory Directed Research and Development Program; Other = some other funding source; NSF/NIH = National Science Foundation of National Institutes of Health; DoD = Department of Defense; DOE-non-SC/non-NW = DOE with some non-SC or non-NW attribution. (Right) Table of cumulative numbers and fractions of articles supported by various funding sources.

Institut in Germany) and Leroy Haggmark (Sandia National Laboratories) in 1980. [23] This article provided the formalism underlying the widely used computer program, "TRansport of Ions in Matter" (TRIM), [24] used to calculate ion range and damage distributions in matter as well as angular and energy distributions of backscattered and transmitted ions. TRIM remains an essential tool for understanding ion/matter interactions in structural materials and has greatly aided the development of electronic materials processing (e.g., CMOS electronics). The underlying journal article has been cited more than 3,500 times, and is currently Sandia's second most highly cited article. An earlier related paper, [25] by Bill Wilson, Leroy Haggmark and Jochim Biersack, has been cited more than 550 times.

Embedded Atom Method (EAM). The second article, by Murray Daw and Mike Baskes (both from Sandia National Laboratories) in 1983, discusses the embedded atom method.[26] Through a first-principles quantum mechanical framework that accounts for, but simplifies, the calculation of many-body effects, this method enabled the quantitative and practical calculation of many basic properties of realistic metals including cohesion, deformation, embrittlement and fracture, as well as calculation of the energetics and geometries of defects and impurities in these materials. A motivating factor for this work was to understand hydrogen embrittlement of steel for Sandia's nuclear weapons mission, but the research was funded by Basic Energy Sciences to develop a more accurate way to describe the interactions in a wider range of metals and alloys. The EAM method became the standard for modeling face-centered cubic metals, and later was extended to body-centered cubic materials and semiconductors.

[23] JP Biersack and LG Haggmark, "A Monte Carlo computer program for the transport of energetic ions in amorphous targets," Nuclear Instruments and Methods **174**, 257-69 (1980).

[24] J Ziegler, SRIM (The Stopping and Range of Ions in Matter) and TRIM (The Transport of Ions in Matter), website (http://www.srim.org/).

[25] WD Wilson, LG Haggmark and JP Biersack, "Calculations of nuclear stopping, ranges, and straggling in low-energy region," Physical Review **B 15**, 2458-2468 (1977).

[26] MS Daw and MI Baskes, "Embedded-atom method: derivation and application to impurities, surfaces, and other defects in metals," Physical Review B (Condensed Matter) **29**, 6443-53 (1984).

The article has been cited over 2,700 times; in addition, two closely related articles (not discussed here) have been cited over 1,000 times.

Nitrogen Chemistry. The third article, by James Miller (Sandia National Laboratories) and Craig Bowman (Stanford University) in 1989, is on the chemical reactions of nitrogen compounds that occur in combustion processes.[27] These reactions were, and continue to be, of great interest because of the impact of various nitrogen compounds (e.g., NO_2 and NO) emitted by internal combustion engines as pollutants into the environment. The article reviewed and synthesized a massive amount of experimental data and theoretical studies, from Sandia National Laboratories and other groups, into a self-consistent, unified, and explanatory set of reactions applicable over a broad range of temperatures, pressures, stoichiometries and fuel types. This article continues to be the basis for our understanding of nitrogen chemistry, and has been cited more than 1,400 times. It has been said of James Miller, a key driving force behind this and related articles, that "it is amazing that a researcher, on the basis of deep insights into physical chemistry, can have such a great impact on such a practically oriented group as the combustion community."[28]

Docking of ligands to macromolecules (AutoDock). The fourth article, by Garrett Morris, David Goddsell, Ruth Huey, Arthur Olson (all from the Scripps Research Institute), Robert Halliday (Hewlett-Packard), William Hart (Sandia National Laboratories), and Richard Belew (UC San Diego) in 1998, is on a method for predicting the bound conformations of flexible ligands to macromolecular receptors, and for computing the ligand-receptor binding affinities.[29] This method makes use of a novel global-local search algorithm based on Lamarckian genetics, combined with a new empirical free energy function. The method has been implemented in the AutoDock software package, widely used in the structure-based drug design community. Like the TRIM software package mentioned above, this is an example where new fundamental understanding, when incorporated into user-friendly computational tools, can have an extremely wide impact on both science and an applications community. Although this article was published within the last decade and a half, it has already accumulated over 2,700 citations.

Evaporation-Induced Self-Assembly (EISA). The fifth article, by Jeffrey Brinker (Sandia National Laboratories and University of New Mexico), Yunfeng Lu (Sandia National Laboratories), Alan Sellinger (Canon Research) and Hongyou Fan (University of New Mexico) in 1999, pioneered a simple new method for self-assembly of nanostructures, along with a fundamental and intuitive understanding of how the process occurs.[30] This method is based on evaporation of a complex fluid in which surfactants and various hydrophilic and hydrophobic constituents are dissolved. Evaporation drives the fluid through various thermodynamic phase boundaries associated with critical surfactant concentrations, ultimately driving formation and then self-assembly of micelles into liquid-crystalline mesophases. The method is compatible with any evaporation-driven process (including spin-coating, inkjet printing, aerosol processing, and dip coating), and hence is a simple, general means for preparing porous thin-film nanostructures as well as hybrid organic-inorganic nanocomposites. Although this article was published within the last eleven years, it has already accumulated over 750 citations, while the accumulated body [31] of EISA-related work has

[27] JA Miller and CT Bowman, "Mechanism and modeling of nitrogen chemistry in combustion," Progress in Energy and Combustion Science **15**, 287-338 (1989).

[28] RJ Kee, P Glarborg, SJ Klippenstein and CA Taatjes, "Tribute to James A Miller," J Phys Chem A **111**, 3673-3675 (2007).

[29] GM Morris, DS Goodsell, RS Halliday, R Huey, WE Hart, RK Belew, and AJ Olson, "Automated docking using a Lamarckian genetic algorithm and an empirical binding free energy function," Journal of Computational Chemistry **19**, 1639-62 (1998).

[30] CJ Brinker, YF Lu, A Sellinger, and HY Fan, "Evaporation-induced self-assembly: nanostructures made easy," Advanced Materials **11**, 579-585 (1999).

[31] CJ Brinker, YF Lu, A Sellinger, and HY Fan, "Evaporation-induced self-assembly: nanostructures made easy," Advanced Materials **11**, 579-585 (1999);

DA Doshi, NK Huesing, MC Lu, HY Fan, YF Lu, K Simmons-Potter, BG Potter, AJ Hurd, and CJ Brinker, "Optically, defined multifunctional patterning of photosensitive thin-film silica mesophases," Science **290**, 107-111 (2000);

HY Fan, YF Lu, A Stump, ST Reed, T Baer, R Schunk, V Perez-Luna, GP Lopez, and CJ Brinker, "Rapid prototyping of patterned functional nanostructures," Nature **405**, 56-60 (2000);

HY Fan, K Yang, DM Boye, T Sigmon, KJ Malloy, HF Xu, GP Lopez, and CJ Brinker, "Self-assembly of ordered, robust, three-dimensional gold nanocrystal/silica arrays," Science **304**, 567-571 (2004);

YF Lu, HY Fan, N Doke, DA Loy, RA Assink, DA LaVan, and CJ Brinker, "Evaporation-induced self-assembly of hybrid bridged silsesquioxane film and particulate mesophases with integral organic functionality," Journal of the American Chemical Society **122**, 5258-5261 (2000);

YF Lu, HY Fan, A Stump, TL Ward, T Rieker, and CJ Brinker, "Aerosol-assisted self-assembly of mesostructured spherical nanoparticles," Nature 398, 223-226 (1999);

YF Lu, R Ganguli, CA Drewien, MT Anderson, CJ Brinker, WL Gong, YX Guo, H Soyez, B Dunn, MH Huang, and JI Zink, collectively accumulated over 3,500 citations. For this and other work, Jeffrey Brinker was awarded an E.O. Lawrence award in 2002 "for his innovations in sol-gel chemistry to create nanostructured materials that have applications to energy, manufacturing, defense and medicine."

ZnO Nanostructures. The sixth article, by Zhengrong Tian, James Voigt, Jun Liu, Bonnie Mckenzie, Matthew Mcdermott and Mark Rodriguez (all from Sandia National Laboratories) and Hiromi Konishi and Huifang Xu (both from the University of New Mexico) in 2003, pioneered a simple, solution-based approach for the preparation of complex, oriented nanostructures in ZnO, a materials system of intense interest for a number of micromechanical, optoelectronic, electronic, and sensing applications.[32]

The approach is based on dip coating a substrate with dense ZnO nanoparticle seeds, followed by growth of those seeds in a solution containing selective adsorbate growth inhibitors to form highly oriented ZnO nanorod arrays. Through systematic variation of nucleation and growth conditions, nanorod morphologies could be varied from nanocolumns to nanoplates, suggestive of biomineral microstructures found in nature. Although the article was published within the past eight years, it has already accumulated nearly 500 citations.

4 Four Case Studies

The previous section highlighted six exceptionally cited contributions to science that Sandia has made through Office of Science support. As mentioned, each of the six represents some beneficial interaction between science and technology, either in both synergistic directions or in one direction. These contributions are all also part of larger program areas, within which additional synergies between science and technology can be found.

In the following four subsections, we discuss in more depth four of these program areas, with an emphasis on the synergies between science and technology, as well as the ways in which both science and technology have been of benefit to mission or societal use.

4.1 Ion-Solid Interactions

The area of ion-solid interactions was Sandia's first Office of Science program. Its origin is discussed in Fred Vook's reminiscences of Sandia's activities in solid-state science.[33] Briefly, the migration of electronics technology in nuclear weapons systems from vacuum tubes to semiconductors brought with it an intense interest in the effects of radiation on the short- and long-term functionality of those semiconductors. The possibility that radiation, particularly bursts from nearby nuclear weapons detonations, might adversely affect weapon electronics functionality was (and continues to be) a significant issue for nuclear weapon surety (safety, security, reliability and control).[34]

As a consequence, by 1958, Sandia had already begun to invest in van de Graaff generators for the irradiation of solids with high energy charged particles. The initial interest was in irradiation with electrons, but by the mid-1960's it was realized that irradiation with ions could greatly extend these studies, as well as reproduce the displacement of lattice atoms in solids exposed to the radiation from nuclear weapons detonations. Hence, positive-ion accelerators were added to the Sandia facilities.

As illustrated on the left side of Figure 5, accelerated, high-energy ions could be "implanted" in the solid to create tailored depth distributions of particular impurities; they could also displace atoms in the solid, thereby leading to point- or clustered-defects and an altered material microstructure. In addition, these ions could backscatter or induce resonant nuclear reactions; thus, the particles leaving the solid were a measure of the composition and even crystalline quality of the probed solid.

By the early 1970's, Sandia's scientific work in this area, particularly work associated with using

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"Continuous formation of supported cubic and hexagonal mesoporous films by sol gel dip-coating," Nature 389, 364-368 (1997);

YF Lu, Y Yang, A Sellinger, MC Lu, JM Huang, HY Fan, R Haddad, G Lopez, AR Burns, DY Sasaki, J Shelnutt, and CJ Brinker, "Self-assembly of mesoscopically ordered chromatic polydiacetylene/silica nanocomposites," Nature **410**, 913-917 (2001);

A Sellinger, PM Weiss, A Nguyen, YF Lu, RA Assink, WL Gong, and CJ Brinker, "Continuous self-assembly of organic-inorganic nanocomposite coatings that mimic nacre," Nature 394, 256-260 (1998).

[32] ZRR Tian, JA Voigt, J Liu, B McKenzie, MJ McDermott, MA Rodriguez, H Konishi, and HF Xu, "Complex and oriented ZnO nanostructures," Nature Materials **2**, 821-6 (2003).

[33] FL Vook, "Frederick L. Vook and Sandia Solid State Science 1958-1994" (2006), included as Appendix 2 of this report.

[34] In July, 1962, the so-called Starfish Prime exoatmospheric nuclear detonation demonstrated the vulnerability of then-modern microelectronics to radiation exposure (it also helped validate the existence of the Van Allen belts). The AT&T system lost the Telstar 1 satellite, which was launched only three days before the Starfish Prime detonation, thereby nucleating a program in radiation effects under Walter Brown, with Sandia National Laboratories (which was operated by Western Electric in the AT&T system) nucleating a similar program under Fred Vook.

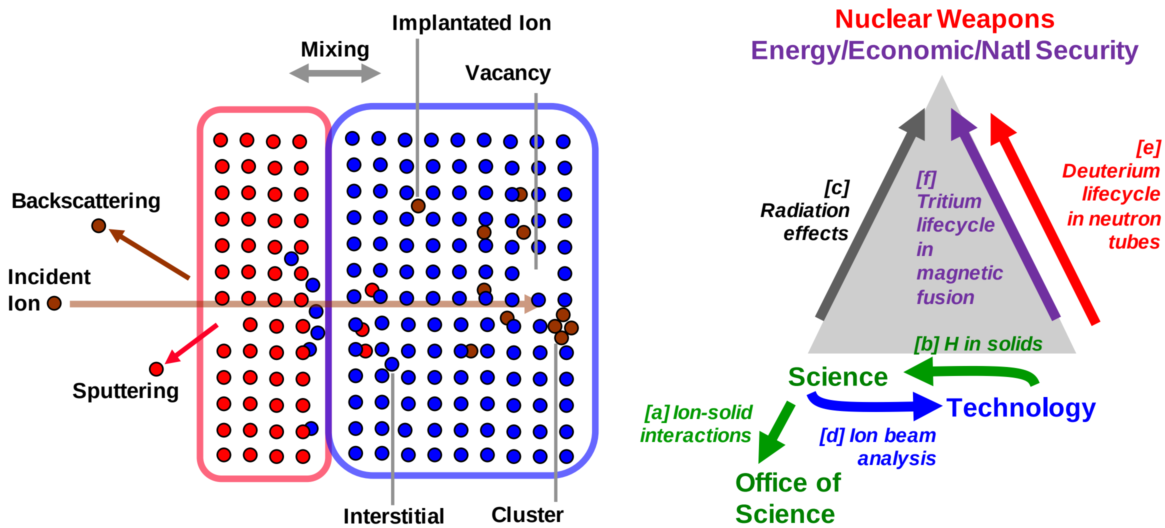

Figure 5: Schematic of physical phenomena associated with ion-solid interactions (left), and examples of science and technology serving various missions related to ion-solid interactions (right).

accelerated ion beams to measure the location of light elements (hydrogen and helium) in heavy matrices (silicon, tungsten, chromium), had attracted the attention of the Atomic Energy Commission's Division of Physical Research (which later became folded into the Energy Research and Development Administration and ultimately the current Department of Energy Office of Science). Sandia was encouraged to submit a proposal, which spawned Sandia's first Office of Science program, on ion-solid interactions, in 1974 (labeled [a] in Figure 5). By the late 1980's, Sandia had built a large body of work in this area, recognized in 1990 when Tom Picraux was awarded an E.O. Lawrence award "for developments in ion-channeling and related ion-beam techniques for materials characterization, leading to new microscopic understanding of materials."

As was true for many of the program areas ultimately supported by the Office of Science, this program benefited significantly from synergies between science and technology. These synergies enhanced the scientific impact valued by the Office of Science, and also benefited Sandia's nuclear weapons and other missions. Some of these synergies are illustrated on the right side of Figure 5, and we briefly discuss these next.

Technology ➔ Science

As mentioned above, charged-particle accelerators enabled an unprecedented degree of control in placing atoms of a particular type, and in producing defects of a particular density inside a solid (ion implantation and ion damage). Near-surface microstructures could thus be tailored to exhibit particular processes or properties of interest. Also mentioned above, charged-particle accelerators enabled non-destructive measurement of the depth profiles of implanted atoms. Taken together, these two capabilities enabled the creation of tailored (and often metastable) near-surface microstructures, the monitoring of their subsequent evolution, and the unraveling of microscopic mechanisms underlying that evolution. These kinds of studies came to be known as implantation metallurgy, and were themselves part of a broad area of study known as materials modification and metastable materials synthesis, a major component of the Office of Basic Energy Sciences' program in the late 1970's.

An example of this work is the study of hydrogen in solids (labeled [b] in Figure 5), an avenue of investigation that has been pursued for several decades at Sandia. This area is of broad scientific interest because an understanding of hydrogen, the simplest prototypical reactive interstitial solute in a solid, is foundational to a similar understanding of a wide range of more complex reactive interstitial solutes in solids.

Moreover, as this work was extended from the study of hydrogen in metals to the interaction of hydrogen with defects in solids, and ultimately to the study of hydrogen in semiconductors, it has become an important foundational element in the much larger field of defects in solids. Through systematic studies, relying on tools both from the field of ion-solid interactions and from a variety of other fields, it became possible to unravel in some detail the energetics and kinetics of transport, interaction, and annihilation/release of hydrogen and its complexes with defects.[35]

[35] SM Myers, MI Baskes, HK Birnbaum, JW Corbett, GG Deleo, SK Estreicher, EE Haller, P Jena, NM Johnson, R Kirchheim, SJ Pearton, and MJ Stavola, "Hydrogen interactions with defects in crystalline solids," Reviews of Modern Physics **64**, 559-617 (1992).

Science ➔ Mission

As discussed above, an understanding of defects, particularly in semiconductors, has helped build a deeper understanding of the effects of neutron radiation on semiconductor electronics (labeled [c] in Figure 5). Though an empirical understanding for a narrow range of semiconductor devices and radiation environments has been extremely important for device qualification, the emerging scientific understanding of underlying microscopic phenomena has helped guide that empirical understanding, and allowed prediction over a wider range of semiconductor device types and radiation environments than would otherwise be practical.

Indeed, with recent decisions to phase out large neutron sources that have been used to develop such an empirical understanding, efforts to develop ever-more-accurate predictive understanding of radiation effects have taken on greater urgency. In 2004, a nuclear-weapons-sponsored program called "Qualification Alternatives to the Sandia Pulsed Reactor"[36] (QASPR) was initiated, aimed at building on foundational knowledge of defects in silicon to develop methodologies for qualifying devices without the requirement of testing in large-scale neutron sources.

QASPR is an ongoing program with two central elements. The first is the identification, understanding, and quantitative mechanistic description of relevant physical processes involving the formation, transport, and reactions of irradiation defects and carriers in bipolar devices, with *ab-initio* theory and experiments being carried out to address gaps in existing knowledge. The second is the establishment of pulsed ion-beam irradiation as a quantitative tool for assessing fast-transient neutron effects in Si and III-V devices, with mechanistic understanding serving to optimize the ion-beam treatments and account for the remaining differences from neutrons. Progress in both of these areas was made possible by the scientific understanding of defects and defect evolution supported over several decades by the Office of Science.

Science ➔ Technology

In parallel with the use of ion-beam technologies to enable science, the science of ion-solid interactions has had a profound impact on new tools and technologies (labeled [d] in Figure 5).

One of the earliest, and still one of the most important, examples stemmed from our deepening *microscopic* understanding of ion-solid interactions. From this understanding, new analytical formulae for determining nuclear scattering angles were developed, which in turn enabled much more efficient methods for calculating the slowing and scattering of energetic ions in a solid.[37] As discussed above in connection with Sandia's exceptionally highly cited articles, these methods were embodied in a widely used computer program called "TRansport of Ions in Matter" (TRIM), a program which to this day is used worldwide as a workhorse tool to calculate ion range and damage distributions, as well as angular and energy distributions of backscattered and transmitted ions.[38]

Another important example is the development of methods for using ion beams to depth-profile increasingly wider ranges of impurities. Among these, Sandia developed a technique called elastic recoil detection (ERD) for hydrogen profiling.[39] This technique made use of forward elastic recoils rather than nuclear reactions, and had simultaneous sensitivity to all hydrogen isotopes. It was also compatible with much more common and convenient low-energy (rather than high-energy) accelerators, and hence could be applied in many more laboratories around the world.

Technology ➔ Mission

Indeed, this ability to measure, non-destructively, depth-profiles of hydrogen and its isotopes in the near surface has been especially important for neutron tubes, an essential component that supplies 14 MeV fusion neutrons to trigger the primary of a nuclear weapon. Neutron tube operation is based on deuterium + tritium nuclear reactions, and deuterium "gettering" and "regettering" in the tube over the course of many shots is a critical determinant of the life reliability of the tube. Because of the ease with which ion beams can be used to measure near-surface deuterium, and because the measurement is non-destructive, ion beam analysis became, and continues to be, a key element in the qualification of neutron tubes (labeled [e] in Figure 5).

Finally, we mention an example in which the ability to measure depth profiles of hydrogen and its isotopes in the near surface has had impact on areas

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[36] This program is discussed in Appendix 3, Samuel M. Myers' "Impact of BES research on national security: Fast-transient neutron irradiation of electronics" (February 8, 2011 revision).

[37] JP Biersack and LG Haggmark, "A Monte Carlo computer program for the transport of energetic ions in amorphous targets," Nuclear Instruments and Methods **174**, 257-69 (1980).

[38] Particle Interactions with Matter website (http://www.srim.org/).

[39] BL Doyle and PS Peercy, "Technique for profiling ^{1}H with 2.5-MeV Van de Graaff accelerators," Applied Physics Letters **34**, 811-813 (1979).

outside of nuclear weapons—in particular, on controlled nuclear fusion. Such fusion is still considered the holy grail of energy sources because of the ubiquity and cleanliness of its fuel, composed of hydrogen and its isotopes.

There are a number of technological approaches being explored for controlled nuclear fusion, and one of the most prominent, particularly from the mid-1970's through the 1980's, was through magnetic confinement of high-energy, high-density plasmas. Because the primary confinement of the plasma by magnetic fields is not perfect, there must also be secondary confinement of the plasma by a solid wall. Sandia played a prominent role in understanding two important aspects of the plasma interactions with the wall (labeled [f] in Figure 5).

A first aspect involved the measurement of depth profiles of the hydrogen isotopes in the wall, and the demonstration that from these profiles could be inferred the energy distribution of ions at the plasma edge. In partnership with the Princeton Plasma Physics Laboratory, deuterium depth profiles were developed into a routine method for inferring tokamak edge-energy distributions, and then used in major tokamak campaigns of the day, providing insight both into plasma edge behavior and into the design of limiters at the plasma edge with minimal erosion.

A second aspect involved hydrogen retention and permeation in the materials selected for the first wall of tokamaks. The choice of wall material is critical, as it controls the implantation, storage, and release of tritium in the wall. Tritium is one of the key participants in the fusion reaction, but also one with high radiation toxicity and hazardous to keep onsite in more-than-tiny quantities. Using insights from laboratory studies of the interactions of energetic hydrogen with materials, as well as from ion beam analyses of test coupons and entire components removed from the Princeton TFTR and other tokamaks, an experimental plan giving a tritium inventory that met environmental and operational constraints was designed. The subsequent successful TFTR d-t campaign and experimentally observed tritium inventory were in close agreement with the predictions. These insights led to designs (e.g., using graphite coatings) that are now standard in state-of-the-art reactors such as the International Thermonuclear Experimental Reactor (ITER).[40]

[40] G Federici, CH Skinner, JN Brooks, JP Coad, C Grisolia, AA Haasz, A Hassanein, V Philipps, CS Pitcher, J Roth, WR Wampler, and DG Whyte, "Plasma-material interactions in current tokamaks and their implications for next step fusion reactors," Nuclear Fusion **41**, 1967-2137 (2001).

4.2 Combustion Science

A second Office of Science program area which we highlight here is combustion science. Sandia's research in combustion science began in 1976, and was another of the earliest of Sandia's programs supported by the Office of Science. Its origin had two motivations.[41]

First, for Sandia's nuclear weapons mission, researchers had been developing tools (particularly laser diagnostics and computer modeling) for monitoring the transient mixing of deuterium-tritium gases (labeled [a] in Figure 6). This mixing is a key process in the operation of nuclear weapons, and was important to understand for potential new weapon designs. Gas mixing is also a key process in combustion and, as mentioned earlier, combustion processes were an area identified as early as 1957 as being of interest to the nuclear weapons program.

Second, during the early 1970's, the country was experiencing an energy crisis. The oil embargo by the Organization of Petroleum Exporting Countries (OPEC), long lines at gasoline stations, and rationing caused the nation to direct its priorities toward reducing dependence on imported oil and improving the energy efficiency of automobiles. It was soon realized that the laser diagnostics and computer modeling tools developed for nuclear weapons purposes could also be fruitfully applied to studying the complexities of combustion (labeled [b] in Figure 6). Better knowledge of combustion processes could lead to more efficient and cleaner conversion of fuels to energy. At the time, automotive engineers did not have tools like lasers and supercomputers, and there was little detailed information about combustion processes.

These motivations led to a proposal for a combustion science program at Sandia to the Atomic Energy Commission, which later became the Energy Research and Development Administration and ultimately the Department of Energy. The proposal led to the establishment of the Combustion Research Facility (CRF), which opened in 1980 and was expanded significantly in a second phase completed in 1999. Most recently an 8000-square-foot computation and visualization laboratory was opened in 2011. The CRF currently represents an 82,000-square-foot facility with 36 individual laboratories, and is operated as a collaborative research facility for the Office of Basic Energy Sciences. Unlike most of Sandia's other research facilities, the CRF is located

[41] RP Carlisle, DJ Monetta, and WL Sparks, *The Combustion Research Facility: Model for a 21st-Century Open User Facility* (Sandia National Laboratories (SAND2001-3742P), 2002).

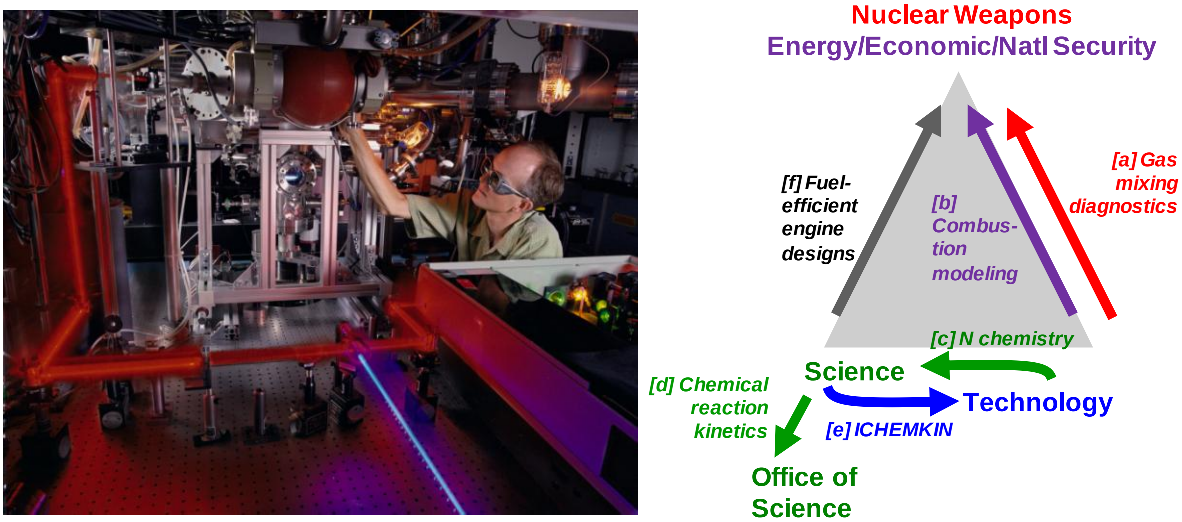

Figure 6: Photo of advanced laser diagnostics used to probe combustion phenomena (left), and examples of science and technology serving various missions related to combustion science (right).

outside classified weapon development areas, and hence is able to host and collaborate easily and actively with researchers from industry and universities all over the world.

Over the years, CRF science and technology have shown the same intertwining and mutual benefit discussed above in the context of ion-solid interactions, as illustrated on the right side of Figure 6.

Technology ➔ Science

The existence of laser diagnostics and computer modeling capabilities were a key impetus for forming a combustion science program at Sandia. These capabilities have indeed played a crucial role in unraveling chemistries of fundamental importance to combustion.

Among these, one of the most important has been the chemical reactions of nitrogen compounds (labeled [c] in Figure 6). As discussed above in connection with Sandia's exceptionally highly cited articles, these reactions were, and continue to be, of great interest because of the impact of various nitrogen compounds (e.g., NO_2 and NO) emitted by internal combustion engines as pollutants into the environment. By 1989, after roughly a decade of work, Sandia was in a position to review and synthesize a massive amount of (its own and others') experimental data and theoretical studies into a unified set of nitrogen reactions applicable over a broad range of temperatures, pressures, stoichiometries and fuel types. The resulting article[42] continues to be the basis for the scientific understanding of nitrogen combustion chemistry, and has been cited more than 1,000 times.[43]

Moreover, this work on the chemical reactions of nitrogen compounds is just the most highly cited and visible example of an integrated approach to chemical reaction kinetics, one that combines theory with sophisticated diagnostics and computer modeling. This integrated approach has benefited in a very general way the rich and large field of chemical reaction kinetics (labeled [d] in Figure 6). For example, it revealed, early on, a need for the heats of formation of free radicals and potential energy barriers to chemical reactions with chemical (1-2 kcal/mole) accuracies. Such quantities are extremely difficult to measure directly (particularly to these accuracies), but are often critical to quantifying a chemical reaction containing a system of elementary steps, many of which involve free radicals as well as potential energy barriers. Through use of sophisticated *ab initio* electronic structure calculations on modern supercomputers, however, it was shown possible to calculate these quantities, and several of Sandia's most cited papers are in this area.[44]

Science ➔ Technology

In parallel with the use of laser diagnostic and computational tools to further a scientific understanding of combustion, the demands of

[42] JA Miller and CT Bowman, "Mechanism and modeling of nitrogen chemistry in combustion," Progress in Energy and Combustion Science **15**, 287-338 (1989).

[43] RJ Kee, P Glarborg, SJ Klippenstein, and CA Taatjes, "Tribute to James A. Miller," Journal of Physical Chemistry a **111**, 3673-+ (2007).

[44] P Ho, ME Coltrin, JS Binkley, and CF Melius, "A theoretical study of the heats of formation of SiH_n, $SiCl_n$, and SiH_nCl_m compounds," Journal of Physical Chemistry **89**, 4647-54 (1985).

studying combustion science spurred the development of new tools for implementing and testing that understanding. Among these, one of the most influential has been a software suite known as CHEMKIN (labeled [e] in Figure 6), which was developed with support from a number of sponsors including BES/CSGB. CHEMKIN is a system of subroutines and databases that can be used to compute all the basic differential equations that describe the time evolution of a gas-phase chemical reaction, regardless of its complexity. Because of the general and open architecture of CHEMKIN, and because of its robust foundation in combustion science, it has come to be used extensively in a wide range of problems involving chemically reacting fluid flow: combustion, of course, but also chemical vapor deposition and chemicals manufacturing. The internal Sandia report [45] documenting CHEMKIN, along with CHEMKIN-related journal articles, has been cited more than 2,000 times. [46] This software package is so pervasive that reaction mechanisms are exchanged among researchers active in the field simply by exchanging CHEMKIN files. Demand for CHEMKIN was so great that the software is now licensed for development and distribution to a private firm, Reaction Design.

Technology ➔ Mission

Note that CHEMKIN, as with the TRIM software discussed previously, is a general-purpose tool that is used both by the scientific community as it unravels complex chemical reaction chemistries, as well as by the technology community interested in predicting the behavior of chemically reacting fluids in commercial and defense systems in practical use.

Here, we mention a recent (2007) example in which a new fuel-efficient 6.7-liter diesel engine was designed for Cummins, a major U.S. manufacturer of engines for autos and trucks. The design made use of Sandia's detailed, science-based understanding of the entire suite of complex processes that occur during diesel combustion, including: chemical kinetics, complex fluid flow, soot models, plume-wall-flow interactions, diffusion flames, and nitrogen chemistries. The result was unprecedented: a design based solely on science-based computer models, and one that met every design goal including those for fuel efficiency and reduced emissions (labeled [f] in Figure 6).

4.3 Compound Semiconductors

A third Office of Science program area which we highlight here is compound semiconductor science. This program area was motivated in the late 1970's by the unique properties of compound semiconductors beyond those of traditional silicon semiconductors: they can be made more radiation tolerant, they can withstand high-temperature operation, they are efficient light absorbers and emitters for optoelectronic applications, they can be used to fabricate very high speed devices, and they represent a large family of materials whose properties can be tailored for particular applications. The high-temperature operation was of particular interest for electronics that could operate at the temperatures of drill boreholes.

All of these properties are of relevance to nuclear weapons, e.g., for radiation-hard optoelectronics. They are also of interest for various defense, energy and other mission uses, including high-power electronics, optoelectronic and microwave communications, photovoltaics for solar energy conversion, solid-state lighting, and sensing. However, these materials were then in their infancy, and in 1978 Sandia decided to systematically develop and integrate the capabilities necessary for compound semiconductor research: solid-state physics, materials and process science, and device design and fabrication.

These capabilities grew steadily from the purchase of the first molecular beam epitaxy (MBE) system in 1981. By 1989, with the help of $10M from the Defense Advanced Research Projects Agency (DARPA), the Compound Semiconductor Research Laboratory (CSRL), with a 3700-square-foot clean room, was constructed. In 1992, the CSRL had been expanded to include a 5000-square-foot clean room; and in 2006 it was replaced by a much larger clean room that is part of the Microsystems and Engineering Science Applications (MESA) facility.

Office of Science support in this area began in 1980, with programs proposed in epitaxy science, especially strained semiconductors, then a new and controversial kind of semiconductor material, and in the science of chemical vapor deposition, a process of growing interest for the synthesis of both silicon and compound semiconductor structures (labeled [a] in Figure 7).

Science ➔ Mission

The first program, on epitaxy science and strained semiconductors, was motivated by a growing worldwide recognition that ultra-thin layers of compound semiconductors could be synthesized

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[45] TH Jefferson, RJ Kee, and JA Miller, "Chemkin: a General Purpose Problem Independent Transportable Fortran Chemical Kinetics Code Package" (Sandia National Laboratories SAND80-8003, 80) (http://www.prod.sandia.gov/cgi-bin/techlib/access-control.pl/1980/808003.pdf).

[46] Reaction Design website (http://www.reactiondesign.com/lobby/open/index.html).

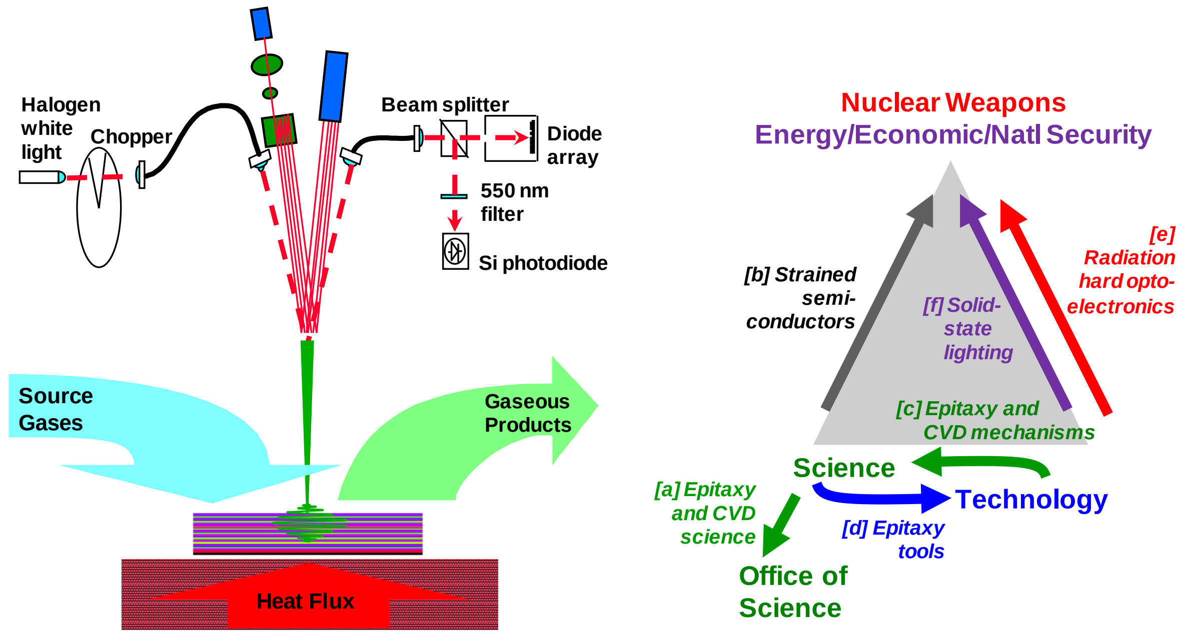

Figure 7: Schematic of advanced laser diagnostics used to probe combustion phenomena (left), and examples of science and technology serving various missions related to compound semiconductors (right).

through new atomic-layer-by-atomic-layer synthesis techniques, including metal-organic chemical vapor deposition (MOCVD) and molecular beam epitaxy (MBE). By combining layers with different alloy compositions (and hence different electronic and optical properties) together into a stacked "epitaxial heterostructure," a number of new physical phenomena could be observed, including ultra-high-mobility electrons and quantum size effects.

At the time, it was nearly universally believed that the various layers in the epitaxial heterostructure needed to have the same atomic lattice constant to within 0.1% to avoid strain induced defects such as dislocations, which would ruin the electronic and optoelectronic properties. However, in 1979, following pioneering work by van der Merwe[47] and by Matthews and Blakeslee,[48] Sandia proposed that high-quality (dislocation-free) heterostructures *could* be made from lattice-mismatched semiconductors, and that the resulting strain could be advantageously tailored to give specific electronic and optoelectronic properties.[49] Then, through emerging synthesis (molecular beam epitaxy (MBE) and metalorganic chemical vapor deposition (MOCVD)) and analysis (including ion channeling, high-resolution x-ray diffraction, and photoluminescence imaging) tools, Sandia demonstrated this concept experimentally.[50]

Subsequent work extended these demonstrations to a detailed understanding of the conditions for stability and metastability of these "strained layer" heterostructures,[51] and to a vast variety of practical devices (labeled [b] in Figure 7). A large fraction of all compound semiconductor devices used today in electronics (e.g., cell phones) and optoelectronics (e.g., lasers for optical communications) incorporate strain in their design to enhance performance.

In 1985, Gordon Osbourn was recognized with an E.O. Lawrence award "for stimulating the new field of strained layer super lattices by making the first theoretical calculations predicting their unique electrical and optical properties."

Finally, we also note that this research went on to fuel significant efforts in nanophotonics and nanoelectronics, and helped lay the foundation for Sandia's role in the formation of the Center for Integrated Nanotechnologies discussed in Section 2.1.

[47] JH van der Merwe, "Crystal interfaces. Part II. Finite overgrowths," Journal of Applied Physics **34**, 123 (1963).

[48] JW Matthews and AE Blakeslee, "Defects in epitaxial multilayers I. Misfit dislocations," Journal of Crystal Growth **27**, 118 (1974).

[49] GC Osbourn, "Strained-layer super-lattices from lattice mismatched materials," Journal of Applied Physics **53**, 1586-1589 (1982).

[50] IJ Fritz, ST Picraux, L Dawson, TJ Drummond, W Laidig, and N Anderson, "Dependence of critical layer thickness on strain for $In_xGa_{1-x}As/GaAs$ strained-layer superlattices," Applied Physics Letters **46**, 967-9 (1985).

[51] BW Dodson and JY Tsao, "Relaxation of strained-layer semiconductor structures via plastic flow," Applied Physics Letters **51**, 1325-7 (1987).

Technology ➔ Science

The second program, on chemical vapor deposition (CVD) science, was motivated by the growing importance of CVD for the synthesis of semiconductor materials and devices.

The initial interest, beginning in 1980, was in CVD processes relevant to silicon. Because of the importance of chemical reactions on surfaces, both in CVD as well as in other reacting fluid flow problems, much foundational work was related to reactions on surfaces: ultra-high-vacuum surface science and molecular beam scattering, as well as the extension of CHEMKIN to Surface CHEMKIN. In addition, a number of *in situ* laser diagnostics were developed in a fashion that mimicked the combustion science area but on a more focused problem: the integration of laser diagnostics and computer modeling to unravel mechanisms for complex chemically reacting fluid flow in such CVD reactors (labeled [c] in Figure 7).

Science ➔ Technology

In the early 1990’s, attention was turned to the increasingly important compound semiconductors, and the far more complex chemistries associated with the MOCVD process used in their synthesis. Optical diagnostic tools were extended so that these processes could be studied in much greater detail and to much greater accuracies. New MOCVD reactor designs, including vertical flow rotating disk reactors in which fluid flow is vastly simplified over conventional horizontal flow reactors, were developed and modeled extensively, and used as experimental research tools for understanding the fundamental physics and chemistry of MOCVD. The simple geometry of these reactors helps one to disentangle the coupled effects of fluid flow and chemistry that is part of all such deposition processes.

The resulting technologies, particularly rotating disk reactors and optical diagnostics, are now used worldwide for the synthesis of advanced compound semiconductor device heterostructures (labeled [d] in Figure 7). Moreover, the accuracies to which these device heterostructures can be synthesized has enabled devices that were previously believed not manufacturable, including the vertical-cavity surface emitting lasers[52] developed in part at Sandia that are now commonplace in high-speed data communications.

Technology ➔ Mission

Finally, we come full circle and note that compound semiconductor devices are now used in existing or proposed nuclear weapons systems, including heterojunction bipolar transistors (HBTs), photoconductive semiconductor switch and HBT Darlington pairs, and radiation-hard photodiodes (labeled [e] in Figure 7). Military systems have benefited even more widely, with compound-semiconductor-based monolithic microwave integrated circuits (MMICs) in high-performance radars.

In addition, compound semiconductor devices are at the heart of an emerging technology, solid-state lighting,[53] with potential energy-to-light conversion efficiencies much higher than those of traditional incandescent, fluorescent and high-intensity discharge lighting (labeled [f] in Figure 7).

4.4 Advanced Computing

A fourth Office of Science program area that we highlight here is supported by the Office of Advanced Scientific Computing Research (ASCR). This area dates back to the early 1950’s when the Atomic Energy Commission, at the urging of John von Neumann, established the Applied Mathematical Sciences (AMS) program. This program ultimately evolved into the Office of Advanced Scientific Computing Research. Among its motivations were the following three:

The first motivation was the most general: a recognition that research in mathematics and algorithms was essential to fully exploit the potential of computing and simulation for both scientific and technological applications.[54]

The second motivation was more specific: the need for modeling and simulation of complex physical processes within nuclear weapons. Indeed, many of the subsequent successes of the AMS program and its successors are of direct consequence to nuclear weapons processes, including the theory and numerical simulation of partial differential equations, computational fluid dynamics, algorithms for solving large systems of linear and nonlinear equations, and methods for modeling and simulating shock waves.

[52] WG Breiland, ME Coltrin, JR Creighton, HQ Hou, HK Moffat and JY Tsao, “AlGaAs OMVPE in a rotating-disk reactor: the anatomy of a VCSEL,” Materials Science and Engineering Reports **R24**, 241 (1999).

[53] JM Phillips, ME Coltrin, MH Crawford, AJ Fischer, MR Krames, R Mueller-Mach, GO Mueller, Y Ohno, LES Rohwer, JA Simmons, and JY Tsao, “Research challenges to ultra-efficient inorganic solid-state lighting,” Laser and Photonic Reviews **1**, 307-333 (2007).

[54] P Colella, D Hitchcock and F Howes, “A Half Century of DOE’s Applied Mathematical Sciences Program’s Contributions to High-Performance Computing,” unpublished.

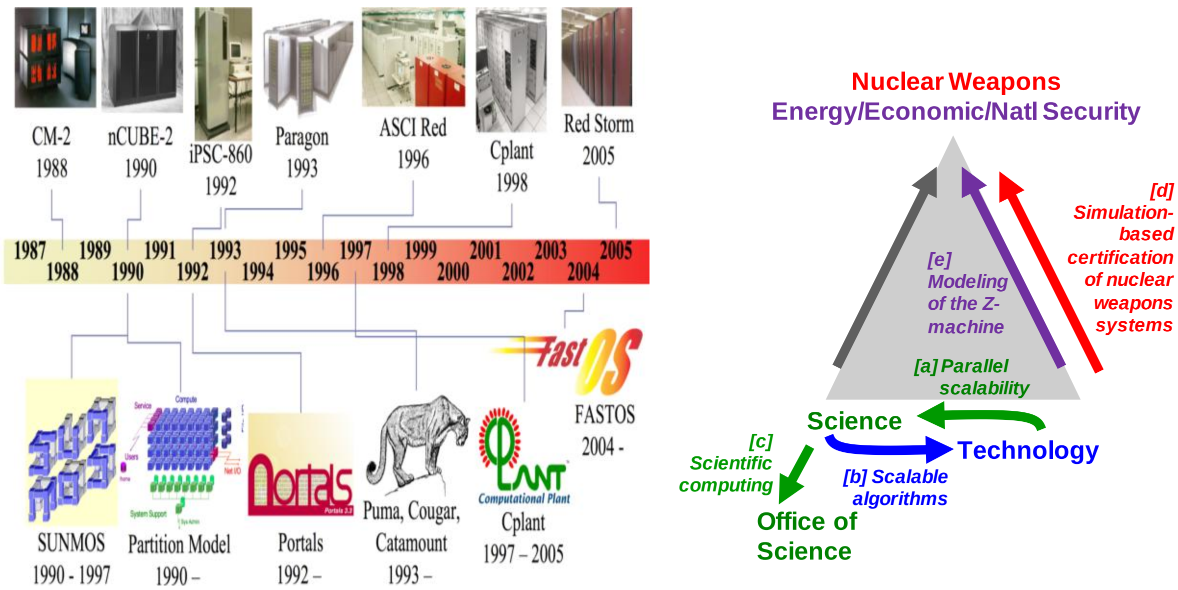

Figure 8: A history of Sandia supercomputers and systems software (left), and examples of science and technology serving various missions related to advanced computing (right).

The third motivation was a desire to take full advantage of the continual improvements in high-performance computing platforms. AMS (and now ASCR) has played a pivotal role in this area as well: from the early days of analog computers; to modern, massively parallel, distributed memory supercomputers; along with advances in the system software required to make these computers usable.

In the mid to late 1980's, Sandia's support from the AMS program (then a part of BES) was modest, with only two projects: one in solvers for ordinary differential equations and one on evaluating special mathematical functions. Internal to Sandia, though, there was an increasing recognition of the importance of advanced scientific computing. A center was formed, with Ed Barsis as director, and a focused effort was made to grow Sandia's support for the Applied Mathematical Sciences program. AMS funding ramped up very quickly, reaching approximately $2M in only a few years. Since then, with focused application-driven programs such as GTL (Genomes to Life) and SciDAC (Scientific Discovery through Advanced Computing), ASCR funding has grown to its current level of approximately $10M/year.

Technology ➔ Science

Much of Sandia's early efforts were focused on acquiring advanced, parallel computing hardware platforms at Sandia, and at the same time developing the operating system, software and algorithmic infrastructure (efforts by Benner, Montry, Gustafson, Womble, and others) to enable effective use of these new computing platforms. Once in place, those parallel computing platforms (considered here as "technologies") could be, and were, used to further two threads of scientific research.

A first thread of scientific research was the mathematics of parallel computation itself. A first example was the mathematics of parallel computing scalability (labeled [a] in Figure 8)—the quantitative amenability of different kinds of problems and algorithms to massive computational parallelization. A second example was the mathematics of graph partitioning—how problems can be partitioned into sub-problems such that the individual sub-problems are about the same size with minimal connections (communications overhead) between them.

A second thread of scientific research was the use of new parallel computing (hardware and software) platforms to solve scientific problems in other fields. A good example of this is the development of MPSalsa,[55] a software project led by John Shadid that developed and made use of a wide range of algorithmic technologies including fully coupled, implicit solution strategies that enabled detailed analysis of three-dimensional, transient, coupled fluid-thermal-mass transport problems with complex chemical reactions (using CHEMKIN). MPSalsa advanced our scientific understanding of a wide range of areas, including: chemical vapor deposition reactors; hydrogen and methane reforming solid-oxide fuel cells; biological systems including defibrillation, cardiac cells, and the

[55] MPSalsa website (http://www.cs.sandia.gov/CRF/MPSalsa).

endoplasmic reticulum; and chemical and biological release and transport.

Science ➔ Technology

Even as the availability of advanced parallel computing hardware and software platforms made possible research on the science and mathematics of parallel computation, the fruits of that research were in turn germinating new Sandia software platforms.

For example, Sandia's research in scalable algorithms (labeled [b] in Figure 8), funded through ASCR's Applied Math Research (AMR) program, ultimately became part of the Aztec Library[56] of parallel, iterative linear solvers (Tuminaro, Heroux, Shadid) which won an R&D100 award in 1997 and seeded the development of the NNSA-ASC funded Trilinos Library.[57] Aztec, and now Trilinos, have in turn had wide-spread impact across both DOE-SC science applications and NNSA mission applications. Aztec, in particular, was a critical component in the success of the DOE-SC supported MPSalsa simulation code mentioned above. Trilinos won an R&D100 award in 2004 and recently became part of the TOPS [Terascale Optimal PDE (partial differential equation] Simulations) Center for Enabling Technology as part of the ASCR SciDAC program.

Or, for example, Sandia's research in graph partitioning ultimately became the basis for algorithms deployed in Chaco[58] (Hendrickson and Leland), later extended under NNSA-ASC to become the Zoltan Library[59] for graph partitioning and dynamic load balancing (Devine, Boman, Hendrickson). This library had impact on a wide range of ASC applications including Xyce for massively parallel electrical circuit simulation and Alegra for simulation of high-energy density physics in the Sandia Z-Machine. Zoltan is now a key component in the ASCR ITAPS (Interoperable Technologies for Advanced Petascale Simulations) SciDAC Center, will soon be fully integrated with Trilinos, and is being used for SC applications including linear accelerator design, astrophysics, climate modeling, and fusion simulation.

Science and Technology ➔ Mission

Over the last three decades, Sandia's programs in advanced computing have had dual and synergistic missions. A first mission was computing for science (i.e. ASCR), with the emphasis on scientific computing as a mathematical/information science unto itself (labeled [c] in Figure 8). A second mission was computing for nuclear weapons needs (i.e. NNSA), as well as impacting Sandia's other missions in energy, and economic and homeland security.

More so than in other areas, the science and technology of advanced computing are tightly intertwined, and in describing the contributions that advanced computing at Sandia has made to its missions, we have not distinguished between them. There are many such contributions; here we mention two of special importance.

A first contribution has been Sandia's joint work with Cray, Inc. on the design and development of the NNSA-RedStorm supercomputer[60] that was one of the most powerful computers in the world (in 2007 #3 on the Top 500 list of supercomputers,[61] now #31). This NNSA-funded system is a critical tool for the NNSA stockpile stewardship mission, particularly as that mission's paradigm has been shifting from test-based to simulation-based certification of the Nation's nuclear weapons stockpile (labeled [d] in Figure 8). Moreover, this supercomputer also led to a successful product line for Cray with more than a dozen systems sold, *and* was also selected as the basis for the DOE-SC ASCR Leadership Computing Facility (LCF) at Oak Ridge National Laboratory (ORNL). This DOE-SC system is currently ranked #2 on the Top 500 and is expected to grow out to a petaflop system over the next year.

A second contribution has been Sandia's use of its algorithmic advances, embodied in open-source libraries such as Trilinos and Zoltan, to model further mission-related problems. Such problems include climate prediction, magnetically confined fusion, automobile tires (with Goodyear), composite structures used for aerospace (with Boeing), chemical lasers (with the Air Force Research Labs), and the Z-machine (labeled [e] in Figure 8). This last problem is of special significance, as it is a major experimental facility at Sandia that is used to explore physics in very high-energy environments with applications to advanced materials and fusion energy systems. Trilinos solvers have been used along with the NNSA Alegra simulator to model critical physical processes occurring in the Z-Machine.

[56] Aztec website (http://www.cs.sandia.gov/CRF/aztec1.html).

[57] Trilinos Project website (http://trilinos.sandia.gov/).

[58] Chaco website (http://www.cs.sandia.gov/~bahendr/chaco.html).

[59] Zoltan website (http://www.cs.sandia.gov/Zoltan).

[60] Red Storm website (http://www.sandia.gov/ASC/redstorm.html).

[61] Top 500 Supercomputer Sites website (http://www.top500.org/lists/2007/06).

5 Closing Thoughts

In this article, we have given a brief history of Sandia's most fundamental science programs – those that came to be supported by the Department of Energy's Office of Science. Although in the early years (1960's through 1980's) support for fundamental science at Sandia from the Office of Science was small compared to that from Sandia's nuclear weapons mission, in more recent years (1990's and 2000's) it has come to be a dominant source of support for fundamental science at Sandia.

We have highlighted in this history those instances where there have been strong and synergistic *direct* flows of knowledge between science, technology and mission. These highlighted instances are of course only the tip of the iceberg. Many more instances have occurred than could be highlighted here. And even more instances in which *indirect* flows of knowledge via outside mediating institutions have occurred than could possibly be highlighted here.[62] Nevertheless, we hope that the instances we have highlighted give a flavor of the Casimir-spiral-like benefits that *can* result from the integration of science, technology and mission within a single institution.

We caution, though, against using this history as an argument that such integration is generally beneficial for a research enterprise. The development of science, technology and mission, and the interaction between these, is always complex. In an increasingly interconnected and "flat" world, in which research institutions scattered across the nation and the world communicate increasingly freely, specialization and division of labor may sometimes be preferable to generalization and integration. Nevertheless, the experience at Sandia has been that generalization and integration are beneficial under the right circumstances, as highlighted here.

[62] These indirect spillovers are a strong argument against insisting too tightly on too direct an impact within an institution.

6 Appendix 1. Richard S. Claassen, "Presentation to MJ Kelley on Fundamental Research at Sandia" (1957)

From: SNL Corporate Archives
Collection # 7, 1100 History of Research
(F. L. Vook) Solid State Science

May 31,

DISTRIBUTION

On March 16, 1957, a presentation was made to M. J. Kelley. It described the plans for "fundamental research" at Sandia. A written form of the presentation by Claassen is attached. His summary of Dr. Kelley's remarks is also included.

Since this program is still in a formative stage, I would appreciate any constructive comments or suggestions on this general subject.

Original signed by
R. S. Claassen

R. S. CLAASSEN - 5133

RSC:frh

Copies to:
G. A. Fowler, 5000
S. C. Hight, 5100
M. L. Merritt, 5110
W. W. Bledsoe, 5120
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MAR 1 6 1957

INTRODUCTION

I would like to describe for you our plans, desires, and goals for a program in what we call fundamental physical sciences. I would like to do this in four parts, following a little background of material. First, I will try to describe the objectives; that is, those accomplishments which we hope to achieve by such a program; second, what I call the configuration of such a group; third, the method by which we have chosen the fields in which we will work; and fourth, two examples of specific programs which have already been initiated in this area.

Since the term "fundamental" and the term "science" are used in so many ways by different people, perhaps we should define first what we mean by "fundamental physical science". The real definition should be evident by the end of my talk, as determined by the boundary conditions we will place on this program and as exemplified by those programs which we can list. Briefly, however, let me say that by "fundamental physical science" we intend to imply research programs which will contribute new and original knowledge of phenomena in the fields of physics, physical chemistry, and to a lesser extent, electrical engineering and engineering mechanics.

As you are aware, Sandia Corporation has reached its present position as a research and development laboratory by a process of evolution. I believe it is pertinent to point out the relationship of this evolving pattern to our present plans for research activities. Originally, Sandia was a split from Los Alamos Laboratories, fostered mainly by geographic considerations. The primary function to be served was that of matching into the military system, and as time went on, to this was added the problem of production of engineering designs which had been partially completed elsewhere. Still later the increased scope of variety of weapons designs has created a logical need for development

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The first objective of this group is that of direct assistance to other individuals in the Corporation. There is an endless variety of circumstances which will bring a technical staff member in the Corporation to the point where he needs advice or information from a specialist in some particular field. We feel that this advice or information is of far greater use to a member of Sandia's engineering staff if it can be obtained from Sandia's own research staff. First of all, there is the matter of convenience and informality. Second, there is a matter of understanding on the part of the specialist of the problems of the Sandia engineer. Third, there is another type of benefit to be gained. The research scientist who is a member of the over-all team of research and development will at times seek ways in which the development engineers or others can achieve better results or reduce their labors for the same end result. This kind of benefit, of course, can be achieved only where the research scientist is working as a member of a team including the development groups, so that he will have continuing access to knowledge of their programs. Perhaps the most important contribution in this first area is that of helping to resolve crises when they arise on the production line, in quality assurance, or elsewhere. A research scientist on our own staff is obviously in the best position to pitch in immediately and help eliminate the problem as rapidly as possible

A second objective for such a group is in the area of new inventions or discoveries. By organizing this group of research individuals as a part of a Corporation, and by proper communication, these individuals should be aware of the various problems facing the Corporation. This knowledge, coupled with their searching into new areas of learning, should from time to time yield inventions or discoveries along lines which might be of use within the Corporation. As we are all aware, inventions are difficult things to come by and cannot be sought directly as such. They can perhaps best be achieved by establishing the proper atmosphere for work by searching minds which are properly loaded with an impedance of known problems needing solutions. Such inventions or discoveries, depending on their particular nature, might well be the starting point or spark to fire up a new program in the applied research group. This then, is another objective of the fundamental physical sciences group.

A third objective is that of specialized but competent advice to management. Such a group as I am describing should have as one of its objectives the recruiting or development of individuals of such stature and ability that they will naturally be sought by management for advice within their particular fields. Many of the important decisions of management in work like ours are highly technical in nature. Since they deal with the future, however, they are not based on cold, statistically analyzed facts, but rather on scientific judgment. It is obviously important that this scientific judgment be formulated by individuals eminently qualified in the field concerned.

A fourth objective of this program is to contribute our fair share to the general fund of scientific knowledge and to the advancement of this fund. To a large extent the Corporation has worked to date by applying to the weapons ordnance business fundamental knowledge which has been acquired elsewhere. If the country is to maintain its lead in the technological weapons race, we must as a nation reach an equilibrium condition where the advances in fundamental technical knowledge balance the rate at which applications can be made to new weapons designs. We feel here that the Corporation has an obligation to make its proportionate contribution to this advance in the fundamental fields. To put this in a different light, we feel that when we go to visit other laboratories, it should be on an exchange basis rather than on a "picking of their brains" sort of basis. This means that we must develop or recruit individuals who stand on equal footing with the others in their field in science.

The fifth objective is a restatement of the first four. The objective is to utilize fully the world of science as it may be applied to the weapons development programs in Sandia Corporation. To make sure that

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we as a corporation are aware of those advances which may be useful in our work, we must have on our own staff research scientists who themselves are contributing to this advance.

The sixth and last objective is that of establishing a rallying point for recruiting and maintaining on our staff the type of individuals required in a vigorous research organization. I believe that such a program or group as I am trying to describe is strongly appealing to research-minded individuals in physics, physical chemistry, electrical engineering, and engineering mechanics. As has been well publicized, there is a shortage of qualified people in these fields. I believe, however, that the advantages in recruiting a strong staff will extend beyond this group itself. I believe that there are many individuals who themselves prefer to work on applications of new knowledge, but who, nevertheless, wish to be closely associated with individuals working in more fundamental areas. In addition to this, it should be an objective of this group to establish to some extent the stature of Sandia as a laboratory. Also, there is an opportunity to establish a espirit d'corps which could be sparked by such a group as this, but which might well extend throughout the research organization and into other parts of the laboratory. In my opinion there is no question but that espirit d'corps is important in holding well-qualified people on the staff.

esprit de corps

2 CONFIGURATION

There are some characteristics of this group which must be defined, and I lump them under the term "configuration"

First, there is the matter of organization in a formal sense. I believe that it is important that such a group be distinguished and, in a sense, protected by an organizational separation from the remainder of the Corporation. Such a group should be an organizational entity so that it is clear both to those within and without the group that this is a set of persons whose primary goal or primary purpose is that of fundamental research.

This brings me to the type of personnel who must be recruited for such a group. They will be comprised of those holding Ph.D.'s in appropriate disciplines, college graduates with lower degrees, and a suitable number of technical assistants. Those individuals who will determine the success or failure of this group, however, will generally be the ones with Ph.D.'s or equivalent talents and interests. It is these individuals who will supply the real initiative and creativeness for the entire group. We must seek out and select those candidates who have the combination of ability, drive, enthusiasm, and interest in research problems. We must search for those individuals who wish to make "research" a career and then give them the proper opportunity to make a success of this career. Generally, such individuals are found by looking at those people who hold Ph.D.'s in physics, physical chemistry, or electrical engineering. In addition, we should make an attempt to recruit some persons who have gone on to post-doctoral research training. Since we are trying to start such a program, pretty much from scratch, we should also look for those individuals who have had active and successful experience elsewhere but who now find their environment changing to a point where opportunity for research is dwindling with their present employer. Such individuals, of course, are hard to find and attract, but on the other hand would be of great value and benefit to such a program.

In addition to a properly protective organization and a staff of properly qualified personnel, I believe that we must establish a proper atmosphere--one which is conducive to effective research work. Atmosphere, of course, is the sum total of many contributing factors. Perhaps the most important factor is an explicit and continuing expression of desire on the part of management for this type of fundamental research. Research people are very gifted and talented along certain lines but after all, they are human and need continual reassurance that they are doing an important job where they are. A natural part of this reassurance of the value of the activity is an establishment of technical objectives which I will come to in a minute. I believe that I would list, next in importance, the freedom of choice on the part of the individual as to the particular problem or program which he will attack. This freedom of choice, of course, is within boundary conditions established by the management of this group in order to channel efforts in those directions which are believed to be most useful to the Corporation. Another factor which is certainly important in establishing the proper atmosphere is that of no time scales and no schedules for these types of programs. Particularly in a place like Sandia Corporation where there is so much emphasis on fast time scales, we must make a special effort to isolate these individuals from the feeling that certain results must be achieved by certain times. As a part of this same problem we must be very careful to avoid the feeling that only success, by way of inventions or discoveries, is rewarded by management in terms of higher salary or standing within the group. Other factors which are important are the provision of the proper types of space and facility, the proper equipment, and what is possibly more difficult to achieve, the proper level of support activities in a business and trade kind of sense in order that the research scientists may give undivided attention to technology and be relieved of worries of an administrative or a business nature. Also, I believe, that we should attempt to achieve the atmosphere of interchange of knowledge as evidenced by local seminars, attendance at scientific meetings, and informal interchange of information with individuals at other laboratories or universities.

CHOICE OF FIELDS

My statements, up to now, have been of a rather general nature. I would like now to describe how we have chosen particular fields for endeavor from among all those available within the physical sciences. This is certainly a most important matter. It establishes the guide

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lines within which the individual scientists will work. The choice of these guide lines is crucial, for if they are wrong, then even the best of research individuals cannot make effective contributions to the Corporation. The choice of technical objectives must be subjected to continual review as the technology changes and as Corporation responsibility changes.

In order to establish initial guide lines, we have made an informal survey of the Corporation activities as they have been in the past and as they are now and as we predict them to be within the foreseeable future. We have tried to look at the large number and wide variety of specific development problems and from these find a kind of set of least common denominators. These are a set of fields or disciplines or sciences which are the underlying basis for the solution of many practical development problems. By this kind of reasoning we hope to establish those fields of endeavor which are most closely related to the various activities within the Corporation as of now and within the foreseeable future.

If we wish to stay somewhere near reality, we naturally cannot include all those fields of physical science which might be of interest to someone in the Corporation. Rather we must choose those fields for which we have some reason to expect a probability of success or contribution. In the process of doing this, we have found it helpful to consider research work as falling into one of two classes. In the one class, there may be a field in which Sandia or the AEC has the only active interest. In this particular field, then, we feel that either we do or support research or else it will not be done. As one example of this type, I might point to stability theory for bluff bodies and, as another example, to three-element triggered spark gaps for very high current discharges. In contrast, the second class contains the areas of research in which there is a vast amount of work being done throughout the country. In these cases Sandia, of course, does not presume to accumulate all the knowledge necessary for its problems but rather to make some contribution in the field and in the process become familiar with the entire field. As an example of this, I might point to the transistor art. There is a great deal of work being done at many institutions as you well know, but we feel that Sandia cannot properly assess all this work and interpret it for our own purposes without having our own individuals active in the field

I have here a chart (Figure 1) which summarizes our thinking to the present time about the guide lines for such a program. I will describe for you, in a minute, two programs which we have started in two of these fields. I might point out first the sort of reasoning which has gone into the divisions shown here. In solid state, for example, there are a number of programs in the Corporation to which this relates. Out of a rather large field of solid-state physics we have a particular interest here in the Corporation in the ferroelectric and ferromagnetic materials. The interest in ferroelectrics derives partly from its use as a contact fuzing element, as a voltage source in some external initiator developments, and its general promising capabilities for many ordnance applications. In addition to this, is the interest in the kinds of applications which Frank Neilson described to you earlier. (Ref.) Ferromagnetic and Ferroelectric One-Shot Explosive-Electric Transducers, Technical Memorandum 230-56-51. We believe that the proposals of Neilson are promising enough and sufficiently different in character to warrant support here at a fundamental level. For the present, at least, this is a field which is of somewhat unique interest to Sandia, or at least to the AEC. On the other hand, however, semiconductors as I have mentioned are of high interest in many places in the country. Because of the continuing reduction in the size of atomic weapons, we expect a steady pressure toward the use of semiconductor devices with their small size and low current drain. The particular research investigations, along the lines of semiconductors, however, can best be determined by the particular individuals whom we are able to recruit for this problem. The important thing here, I believe, is that we have on our own staff a man who is familiar with the field of semiconductors and is well qualified to interpret this field to the Corporation.

As another example, let us look at Theoretical Mechanics. We have a continuing and large problem in shock and vibration, those mechanical environments which place severe requirements on our weapon designs. This problem is common to all military designers but has not been satisfactorily solved by any of us. Some preliminary work which was done here a few years ago has indicated that this problem may be susceptible to partial solution by more detailed theoretical interpretation. A problem which, at the present time, is somewhat unique to Sandia is that of resistance to shock impact for extremely high-g acceleration. The trend toward tougher and tougher warheads, which contain only big lumps of material, is placing an extreme load on the individual components which must be designed by Sandia. These components themselves, because of their particular function, may contain many small and possibly complicated parts. The response of these systems to high shocks or high decelerations is not a thing which can be simply analyzed and is certainly poorly handled by static analysis. We believe that a behaviour of materials such as metals and plastics, at very high rates of stress application, would be a very interesting field for research.

I would like to point out that we have a column entitled "theoretical" and that I believe that this column is quite important. One of the characteristics of a university staff, and I think particularly so of those universities which have been most productive, is a balance between theoretical and experimental scientists. The history of science is pretty much a "leapfrog" sort of pattern in which first theory and then experimental evidence seem to get ahead of the other. I believe that it is only by an interchange of individuals concentrating in theory or experimentation that one achieves the most effective output from a given sized group. I believe that the variety of programs which we have listed here should offer a sufficient challenge for most any theoretician

Note also that we have listed a column which is called "experimental analytical techniques". This is listed separately to emphasize the fact that we expect that such a program will contain as an integral part some research on the analytical procedures themselves where these procedures are done by physical measurements. We intend, of course, to make use of what equipment and apparatus as already available within the corporation. We expect, however, that some of the analysis work will be of such an individual and unique character that it will be a research problem within itself and should be handled within the group.

EXAMPLES

As specific examples of the types of programs we are planning, I would like to talk about radiation effects and physical electronics. Let us deal first with radiation effects. The Corporation is interested in the damaging effect which nuclear radiation may have on materials or components, because of possible vulnerability to enemy counterweapons and, at a time somewhat farther in the future, the damage which may be caused by the radiation environment of a nuclear power plant in an aircraft or a nuclear rocket. This interest has been formalized in a letter which Gen. Hertford from AEC has written to AFSWP in which he states that Sandia Corporation will have the primary responsibility for the AEC in the study of radiation effects on weapons and their components. You have been briefed, I understand, on the comprehensive engineering program which we plan at Sandia to prove out the capability of our weapon designs against radiation. This program will be centered about the reactor facility which is now a part of our budget request.

We here in Research feel that this engineering program should be balanced by a more fundamental program in which individuals on our staff attempt to gain a better understanding of the fundamental processes which are involved in the interaction of nuclear radiation with matter. To get started in this program we have chosen four fields for investigation. First of all are the semiconductors. These are the most sensitive devices to radiation damage and therefore are of most critical interest. We have faith that by one means or another the intolerance of solid-state devices to irradiation damage will be solved as time goes on. Perhaps we will be able to make some contribution to this solution in those areas which are of particular interest to us. We plan to start this program on two levels. On the one hand, we will repeat experiments done elsewhere to establish self-confidence in our techniques and the equipment. At the same time, we will perform experiments in connection with Series Plumbbob to take advantage of the unique source of extremely high rates of neutron exposure.

Second are the polymers and their interaction with radiation. We are fortunate in having on our staff a man who has had experience along these lines at one of the country's major rubber and plastics companies. Polymers are of interest here, of course, for insulation purposes in electrical components and as structural members where low-density material is required.

Third, we plan some work in the area of alkali halides, not so much because of direct application in weapon design, but rather because these materials are relatively simple in structure and there is at least some possibility for theoretical interpretation of the experimental results and potential use in dosimetry.

Fourth, we have already done some preliminary work on the effect of radiation on the ferroelectric materials. This work was done in connection with the Redwing series in the Pacific last year. Because of this start and because of our general interest in the ferroelectrics, we would like to follow this up with further work on the interaction of radiation with the ferroelectric materials. We have hopes that changes here at the crystal structure level may be revealed by external change in the piezo- or ferroelectric properties of these materials.

As the primary experimental facility for this program, we are purchasing a van de Graaff generator and expect to have built a proper building to house this. We have chosen the van de Graaff for its versatility in the types of nuclear particles which it can produce and for its ability to produce particles of one type only and of a known energy or energy spectrum. We believe that this equipment will make a very fine complement to the reactor facility which is planned here. We have also spent a considerable amount of effort and time on the plans for the reactor facility itself. We are anxious to see that these plans, while achieving the primary purpose of providing a test facility, also allow for the effective use of this reactor as a research tool in the study of irradiation damage on materials. To this end we have requested the inclusion of such items as rabbit tubes which go very near the reactor core and even tubes which go inside the boral thermal neutron shield so that we can achieve higher neutron activation on small samples when required. In addition to these facilities, we plan, as I have mentioned, participation in the full-scale tests which are the only source at present of the very high neutron fluxes which might be the final test of our particular designs. As a laboratory substitute for a source of very high fluxes of neutrons, we have considered the use of a Godiva-like critical assembly system which will give neutrons at a very high rate but for a very short duration. Our consideration of this has not progressed beyond the talking stage. We are already convinced, however, that one of the things we must understand is the effect of a rate of exposure upon the damage which may be done. Our primary facility for testing of actual development components will be the reactor in which very high total fluxes can be achieved only by long exposures at moderate flux rates. It is obviously most important to establish whether this kind of a test is fully equivalent to the same total dose delivered in times less than one second.

As a second example of the kind of programs of problems that we propose in a given field, let us look at physical electronics. The Corporation makes extensive use of three-element gaseous discharge tubes in practically all weapon designs, and every weapon containing an implosion warhead depends on exploding wires to initiate its sequence. Many of our weapon designs are now using external neutron sources which are essentially a type of ion tube. In all of these fields, a great deal of empirical work has been done in which various parameters have been correlated with the electrical or energy inputs required.

In the area of exploding wires, George Anderson and Frank Neilson have already done some good work in trying to correlate the physical properties of the wires with their electrical history as they explode. We believe that this type of work is worthwhile in understanding what is going on and that it could be extended to include a study of the interaction between the exploding wire and surrounding PETN. The studies to date have already yielded a sufficiently better understanding of the process involved to allow for a reduction by a factor of ten in the electrical energy required for a detonator to be properly initiated.

Sandia has done or sponsored a great deal of work which has allowed for the design of triggered electrodes and, along somewhat parallel lines, the design of neutron sources. In the one case, we have only a most superficial knowledge of how the triggering spark transfers to the main gap in a trigger electrode switch. In the other case, we have only the poorest understanding of how the source spark actually creates and liberates hydrogen ions into the surrounding atmosphere.

We believe that an investigation into the ion production phenomena might be most rewarding. This type of knowledge may well be overlapping with the work in high temperature. It looks there as though a very high-energy spark gap may well be the most convenient laboratory source of pulsed high-temperature source.

CONCLUSION

These are the first examples of the type of work we would do in fundamental research. We believe that it has direct value to the Corporation and should be supported and expanded.

R. S. Claassen - 5133

RSC:5133:xp

SF 2900-KBS-864

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Physical Sciences Research at Sandia

Source: richard S. Claassen Collection Frank Hudson Collection - Deerived from Hudson's initial plan for Fundamental Research at Sandia

	SOLID STATE	RADIATION EFFECTS	COMBUSTION PROCESSES	PHYSICAL ELECTRONICS	HYDRO- MAGNETICS
PROGRAMS	Semiconductors Ferroelectrics Ferromagnetics	Semiconductors Polymers, Ionic Crystals	Propellants Heat Powders Explosives	Gaseous Discharge Ion Production Exploding Wires	Impluse Tube RF Moving Field Machine
TYPICAL PROBLEMS	Electronic vs. Ionic Nature of Ferroelectricity Relation of Surface Condition to Electrical Properties High Energy Density Properties of Ferroelectrics and Ferromagnetics	Damage Mechanisms in Semiconductors Structural Changes Induced in Polymers Color Centers in Alkali Halides Rate Effects in Neutron Doses	Heat Powder Burning Parameters Study of Transient Gas Products in Explosives Relationship of Structure to Propellant Burning	Energy Propagation in Gaseous Discharge Mechanisms of Ion Production Energy Production and Transfer Related to Exploding Wires	Magnetic Coupling Separation of Ohmic Heating and Magnetic Acceleration Magnetic Structure of Shocks
SANDIA INTEREST	Transistors Diodes Voltage Sources	Vulnerability Radiation Environment	Exploding Switches Thermal Batteries Detonators Propellant Activated Devices	Spark Gaps Switching Tubes Detonators Zipper Sherwood	Sherwood, Fireball Re-Entry High-Temperature Sources

Physical Sciences Research at Sandia

Source: richard S. Claassen Collection Frank Hudson Collection - Deerived from Hudson's initial plan for Fundamental Research at Sandia

HIGH TEMPERATURE	THEORETICAL MECHANICS	GEOPHYSICS	THEORETICAL	ANALYTICAL
Thermal Shock Energy Transfer Material Properties Ablation	Dynamic Similitude Stress-Strain-Time Relationship	Upper Atmosphere Physics		
Effect of Thermal Transients on Surfaces Grain Boundaries Near Melting Ablation in Controlled Atmosphere	Scaling Laws in Dynamic Studies Molecular Structure-Mechanical Property Correlation Strain Produced by Short Duration Stress	Energy Transfer at High Altitudes Altitude Dependence of Various Parameters	Theoretical Physics Support of Other's Research Programs Independent Programs	Development of special Techniques for Detection of Physical Changes and Interpretation of Secondary Indications of Such Changes in Support of Other Research Programs
Fireball Re-Entry Sherwood Rover	Shock & Vibration Model Studies of Warhead Design	High Altitude Systems	Research Support	Research Support

7 Appendix 2. Frederick L. Vook, "Frederick L. Vook and Sandia Solid State Science 1958-1994" (September 26, 2006 revision)

Editor's Note: This Appendix contains a short autobiographical account of Dr. Frederick L. Vook. Dr. Vook was a member and Director of the Solid State Science Directorate during the years when Sandia's major research programs and relationship with the Department of Energy's Office of Science were initiated. The account is written conversationally, hence contains many "first person narrative" details of peripheral interest to this document. However, we include it here as an appendix because of the many important historical details it contains of the development of Sandia's relationship with the Department of Energy's Office of Science.

Preface

This is a short record of my history in the Solid State Science Directorate Org. 1100, from 1958 through 1994. Some of the major research programs and the contributions of key people are reviewed.

I Introduction

In 1942 E.P. Wigner, working at the Manhattan Project, recognized that energetic fission fragments and fast neutrons from nuclear reactions could displace atoms of materials and lead to serious damage. Wartime research by Wigner and Fred Seitz was classified until some fundamental work was published in 1946. Some technological work was published in 1955 as a result of Eisenhower's "Atoms for Peace" program. The interest in defects in solids produced by radiation involved many other noted physicists including Neils Bohr, J. C. Slater, W. Shockley, Harvey Brooks, and A.W. Overhauser.

In the early 1950's Fred Seitz and J.S. Koehler came to the University of Illinois bringing their interest in the solid state physics of radiation damage with them. Koehler's group began using the Illinois cyclotron for radiation damage experiments. In 1956 the publication by Seitz and Koehler of "The Displacement of Atoms during Irradiation" began to place the field on a sound theoretical basis. I joined Koehler's group at Illinois and received my Ph.D. in physics in 1958, on low temperature length change measurements on cyclotron 10 MeV deuteron irradiation of Germanium.

In the 1950's physicists at the University of Illinois, Oak Ridge, and Argonne National Laboratories were among the pioneers of the study of radiation induced defects in solids, primarily metals. Some notable work on semiconductors was also done at Purdue University and at Bell Telephone Labs.

II Sandia 1958

At Sandia interest had begun on the effects of irradiation on nuclear weapons components and in particular on weapon electronics. When I came to Sandia in September of 1958, Dick Claassen and Frank Hudson had already convinced Sandia management that a fundamental understanding of radiation damage was necessary to understand the engineering aspects of Sandia's weapons mission. They had received approval to purchase a 2 MeV Van de Graaff accelerator, which had already been installed in Bldg. 803 when I arrived. Building 803 was located outside the classified security area so that the scientists could interact with uncleared scientists from universities. This accelerator (which I saw on my interview visit to Sandia in the spring of 1958) and the ability to publish my research in the open literature confirmed my interest in coming to Sandia. At this time Sandia had very little recognition in the research community, so that coming to Sandia was not for the faint of heart, and no bright research future was guaranteed.

I actually visited Sandia on an interview visit sponsored by Los Alamos where I had worked several summers earlier. (My work at Los Alamos involved shock wave physics, also of interest to Sandia.) In response to a Sandia ad in Physics Today I called Dick Claassen to suggest that I stop in to Sandia on my visit to Los Alamos. Los Alamos did make me an employment offer in theoretical physics as related to the nuclear rocket program Rover, but I never thought that the nuclear rocket was practical.

My thesis at Illinois involved 10 MeV deuteron irradiation that produced both simple point-defect-like vacancies and interstitial defects but also larger clusters of defects. These point defects are considered the fundamental defects in radiation damage. Previous measurements generally involved electrical measurements such as electrical resistivity and carrier concentration degradation. However, although electrical measurements in semiconductors are very sensitive to defects, they are not at all selective as to the kinds of defects. I was interested in separating the effects of the point defects from those of larger clusters produced mainly by neutron irradiation damage by using length change measurements.

Irradiation with 2 MeV electrons (producing only point defects) using the Sandia Van de Graaff would allow that separation. My results on silicon showed that the major part of the damage produced by deuteron irradiation is indeed caused by large clusters, and very little lattice distortion is caused by point defects. In contrast, my electron irradiation results on the III-V compound semiconductors GaAs and InSb showed large distortions around point defects.

Irradiation of electronic devices or weapon components using macroscopic measurements such as electrical changes are phenomenological measurements, which give information only under the particular conditions of the experiment, but don't provide the necessary microscopic mechanistic information to make predictions for different conditions. Correlation with microscopic fundamental defects helps to provide predictive capability.

At Sandia in Bldg. 803 I set about building a liquid helium irradiation cryostat for low temperature electron irradiation experiments on semiconductors. Low temperature irradiation is necessary to freeze in the defects as produced before they interact with each other or with impurities. Building 803 was a hotbed of cramped activity. My office of 110 square feet was also my lab. I had no lab assistant. The room outside my office was used in common by 5 staff members, 2 staff associates, and 2 staff assistants. There was no usable wall space because the room had 10 doors entering it, a Van de Graaff console, a sink, and an exhaust hood. It was cramped. Also small hand tools were held in common, which meant that they were not easily available. I made myself somewhat of a revolutionary by insisting on having my own tools with my name on them.

The culture in Org. 5150 was interesting. Staff members (mostly new Ph.D.s) had their own research programs, primarily conceived and directed by themselves with little management oversight. Staff members were on their own to make their programs succeed or fail. Funding was not an issue and was sufficient without requiring staff members to seek their individual funding. Use of the accelerator, however, required scheduling and sharing irradiation time. Staff assistants were scarce.

III Sandia Radiation Effects Reorganization 1962

The growing recognition of the importance of radiation effects led to a Sandia reorganization in about 1962. George Dacey, the vice president of Research (5000) consolidated radiation effects research under new director Jim Easley (5200). Both Dacey and Easley came from Bell Labs where radiation effects were of interest to satellite communications. AT&T satellites (e.g. Telstar) bombarded by Van Allan Belt radiation sustained damage to the satellite electronics. The nuclear reactors in Area 5 were also moved under Easley's direction, since they were also used for irradiation experiments. The Area 5 reactor had a very large irradiation room so that it could irradiate a complete weapon. As George Dacey said to a group of visitors, "The room is large enough to irradiate an elephant, hopefully one that isn't white."

I was promoted in 1962 to Division Supervisor of Radiation Effects Research Division under new manager Fridolf Smits, also from Bell Labs, under Jim Easley. The Van de Graaff operation was moved into my division out of Dick Claassen's 5100-research organization to consolidate the radiation damage research under Jim Easley.

IV Radiation Effects Research Results and Recognition

Beginning in 1958, fundamental radiation effects research at Sandia began a long expansion over decades that moved Sandia to international recognition. My Illinois thesis on deuteron irradiation was the subject of an invited paper at the Conference on Radiation Effects in Semiconductors held in Gatlinburg, Tennessee in 1959. In 1962 I presented my new Sandia research at an invited paper at the International Conference on Crystal Lattice Defects in Kyoto, Japan. Presenting research at a foreign international conference was a singular event for a Sandia researcher at that time.

The Sandia results on isolated point defects showed that the previous deuteron results included large effects of clustered defects. I presented additional new research at the International Conference on Radiation Damage in Semiconductors at Royaumont, France in 1964. A memorable occasion was the lavish conference dinner at Versailles with formal wear and liveried footmen.

In my division we were able to focus the research of several staff members (especially Herman Stein, David Brice, Ruth Whan, Keith Brower, Alan Sattler, and George Arnold) on critical questions on the identity of the defects in semiconductors. The focused attention of a group effort was a new mode of organizing research at Sandia and provided a very desirable impact. By combining theoretical calculations and several different experimental measurements at low temperatures with tailored samples having selected impurities our group made considerable progress understanding the stability, identity, and electrical properties of the defects in silicon and germanium.

In 1967 I organized an international conference on Radiation Effects in Semiconductors held at the

Bishops Lodge, NM. President J. A, Hornbeck, Vice presidents R. C. Fletcher and T. B. Cook approved the proposal for the conference. Sandia and the U.S. Atomic Energy Commission supported the conference. Plenum Press, in a book entitled Radiation Effects in Semiconductors edited by myself, published the Proceedings of the conference. Nine Sandians presented invited papers at the conference. Six were from my division, including H. J. Stein, R. E. Whan, A. R. Sattler, D. K Brice, G. W. Arnold, and myself.

The Santa Fe Conference gave new international recognition to our Sandia research. It was an exciting time. George Watkins and James Corbett of the G.E. Research Laboratory had used electron paramagnetic resonance (EPR) and infrared absorption to identify the microscopic structure of many defects in silicon. Keith Brower of our group also discovered new EPR identifications of defects in silicon. These identifications provided keys to determine the precise inventory of defects produced by different kinds of irradiation.

V Ion Implantation and Ion Beam Research, 1967

Two new developments presented at the Santa Fe Conference took our interest in a new but related direction. These were the discovery of ion channeling and the beginning of ion implantation research in semiconductors. Alan Sattler of our group had begun ion-channeling experiments also. At Sandia, interest in radiation effects research in semiconductors for predicting damage to electronics was waning. Upper management thought Sandia knew enough about radiation effects in semiconductors for engineering purposes. (Interest later picked up again and remains of interest even now, 2006)

Bill Shockley, who shared the Nobel Prize in Physics for the invention of the transistor, had proposed an ion implantation process for doping silicon semiconductors to make devices, as a substitute for the normally used diffusion process. Ion implantation has now become the dominant process for making silicon integrated circuits. However, at that time the unwanted effects of the damage produced by the ions defeated the process. Shockley thought that the only defects produced by the ions were simple defects such as interstitial atoms and lattice vacancies, and that annealing could easily recombine them. We, however, thought the defects were more complicated, and could recombine with each other and with impurities to produce unwanted electrically active rather stable defects. Here was an opportunity for Sandia. I took my group together and told them we were going to help solve the ion implantation radiation damage problem. To do that we were going to convert the Van de Graaff accelerator from electrons to ion beams to start implantation experiments. Some people thought this would take a year to get up to speed in a new direction. However, it took only 6 months to produce new meaningful results. Jim Borders, S. Thomas Picraux, and Sam Myers joined our group. We were able to apply our theoretical and experimental techniques from radiation effects in semiconductors to ion implantation damage. Our efforts were quickly rewarded, and Herman Stein, Keith Brower, David Brice, and I were able to determine the identity, stability, and depth distribution of defects produced by ion implantation.

We helped propose the First International Conference on Ion Implantation in Semiconductors that was held in Thousand Oaks, CA in 1970. Five members from my division including myself presented invited papers. Even at that time industry had not yet become a believer in the viability of ion implantation doping for device production. At that conference Gordon Moore, president of Intel, stated that industry was sufficiently comfortable with diffusion doping that they would "never replace diffusion furnaces with ion implant accelerators one to one". Years later when I questioned him about his earlier remarks he said, " well I was right; it’s at least 10 to one".

VI Growth of International Recognition and Promotion to Manager 1971

I was promoted to manager of Radiation Physics Research Department in 1971.The research in ion implantation and ion beam studies of solids grew rapidly over the years. Many international conferences were held. They were held in Garmish, Germany in 1971; in Kyoto, Japan in 1971; in Reading U.K. in 1972; in Osaka, Japan in 1974; in three conferences in 1975 in Warwick, U.K.; Karlsruhe, Germany; and Amsterdam, Netherlands. My group and I gave papers in all these conferences.

As the interest in ion implantation grew, materials other than semiconductors became of interest. In 1973 I promoted S. Tom Picraux, who joined my group in 1967 and with whom I collaborated on many papers, to my Division Supervisor position. Tom, E. P. EerNisse, who was the supervisor of another device division in my department, and I organized an international conference on the application of ion beams to metals. The conference was held in Albuquerque in October 1973. The proceedings entitled, “Applications of Ion Beams to Metals," edited by S. T. Picraux, E.P. EerNisse and F. L. Vook, were published by Plenum Press.

In 1974 the American Physical Society commissioned a study on Radiation Effects on Materials as one of a series on Physics Problems Relating to Energy Technologies. As a result of Sandia’s growing

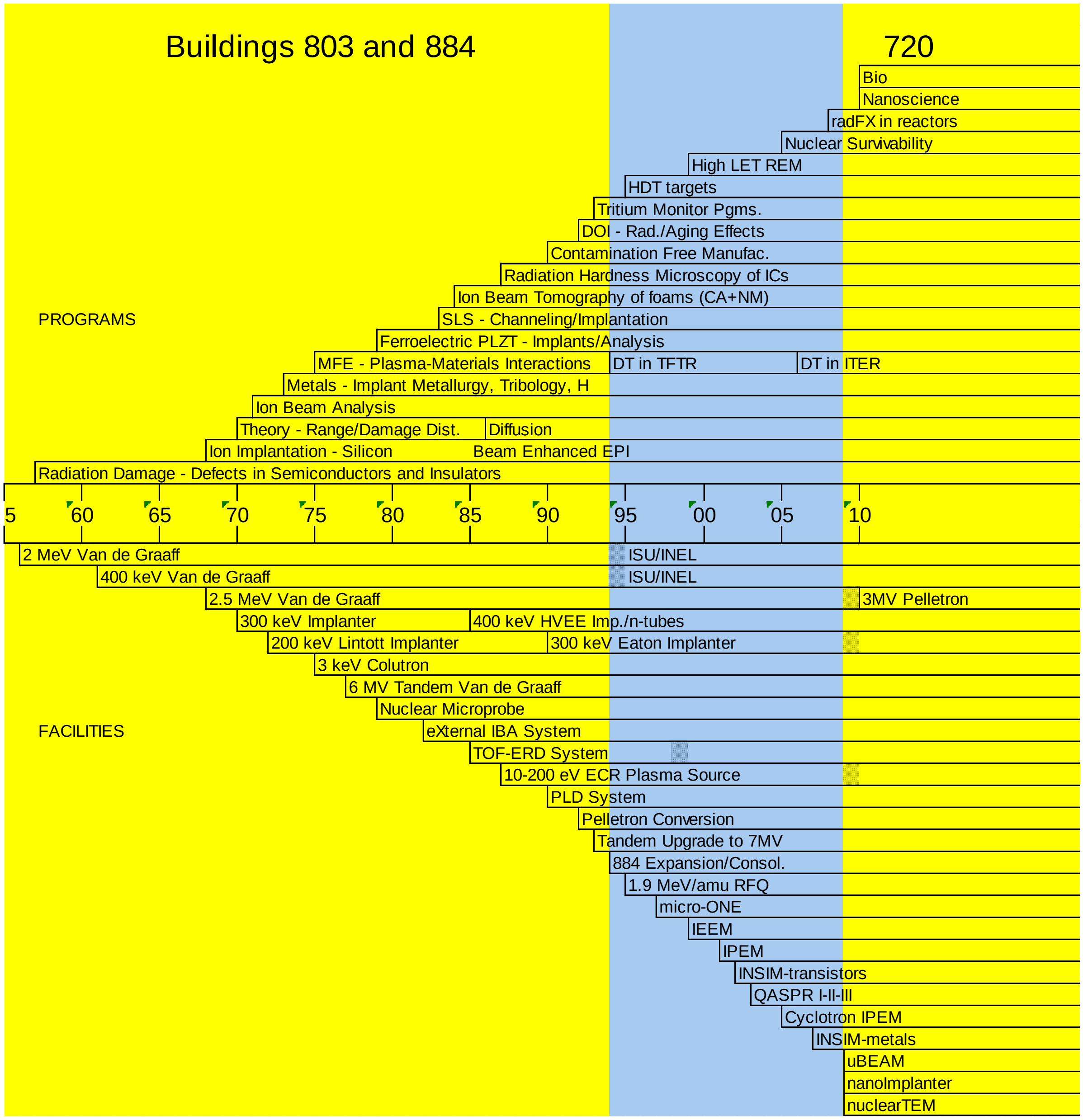

Figure 8-1. Timeline of ion beam research programs (top) and facilities (bottom) over nearly 40 years of Organization 1100 [*Editor's note: the timeline shown here is one updated in 2011 by Barney L. Doyle*]. Some of the accelerators are still actively used today as part of Sandia's Ion Beam Laboratory, completed in 2010.

reputation in this field I was asked to lead and chair a study on the Effects of Radiation on Materials. I wrote an article on the results of the study in Physics Today. The complete report was published in Reviews of Modern Physics. It is interesting particularly today to recall the opening sentences of my 1975 Physics Today article. "The United States is conducting an intensive search for more—and lower cost—energy. Because of its relatively low cost, nuclear energy is rapidly becoming an important source of energy". Subsequently, I participated in a review of the field in 1981 in which a report was published under the auspices of the Council of Materials Sciences for the Division of Materials Sciences of DOE.

In 1976, a special small conference of experts was invited to participate in a conference with scientists of the People's Republic of China. Only six U.S. scientists were involved, including Sandians Dave Brice and myself. President Nixon had recently opened relations with communist China that had prepared the way for this conference. We arrived in China in the one-month period of mourning just after Mao Tse-tung had died. The situation was tense because no one knew who was in charge in China.

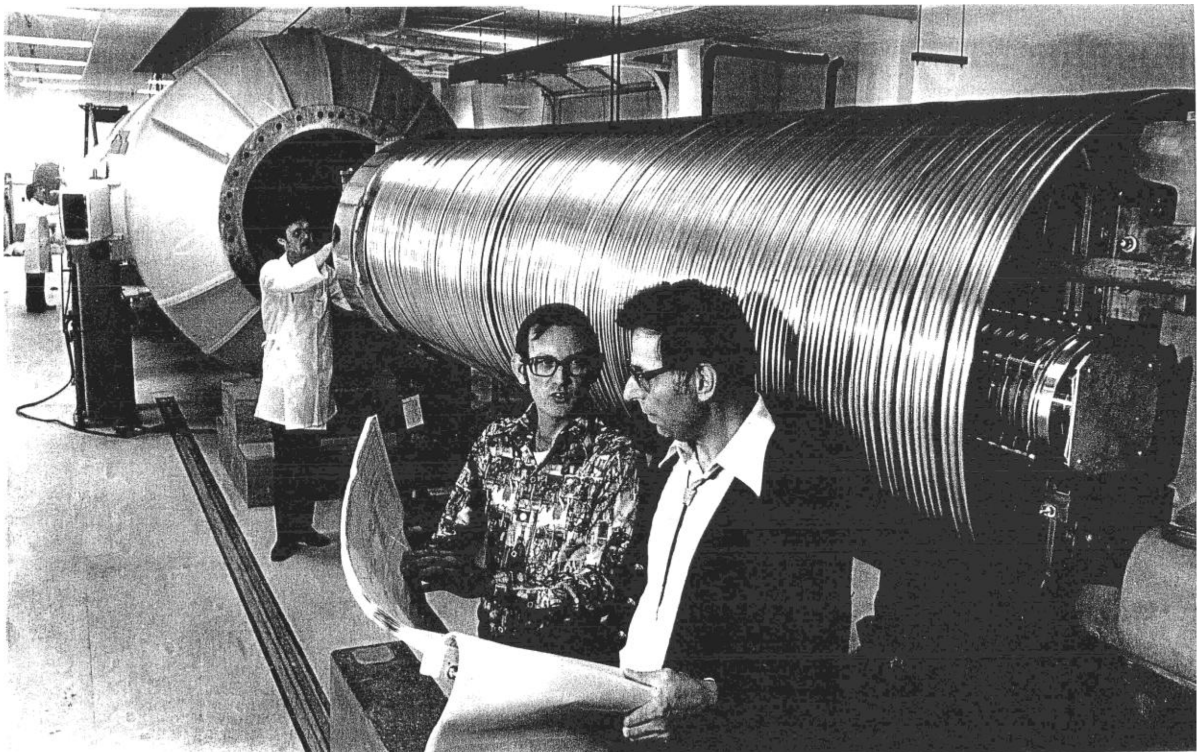

Figure 8-2. A 6MV Tandem Van de Graaff accelerator installed in 1977. From back to front are: Barney Doyle, Norman Wing, Paul Peercy, and Fred Vook.

The man from the Chinese Electronics Society who had arranged the meeting did not meet us when we arrived in Beijing. We learned later that he was "being re-educated". We had taken our wives along and were treated liked visiting dignitaries. Each of the US scientists and their wives were driven in a separate car with driver and interpreter. We visited universities and research labs throughout China including Beijing, Xian, Shanghai, and Hangchow. As we departed Shanghai, street demonstrations had started which led to the end of the Cultural Revolution and the beginning of a somewhat capitalistic China.

VII Promotion to Director of Solid State Sciences (Org. 1100) in 1978

In 1978 I was promoted to Director of Solid State Sciences, Org. 1100. As Director, I had a considerable amount of budget authority under Cases 1 and 2. This budget authority was given to me by the vice president of research, John K. Galt, who was from Bell Labs and preceded me as director of 1100. As vice president of research he was also chairman of the Research Allocation Committee (RAC) and was responsible for the allocation of a considerable amount of weapons research funding. This resulted in fairly stable funding for research in a competitive environment with other research activities. Much later, by 1992, this budget responsibility was removed from the vice president of research. As serious declines in the weapons research funding of 1100 began, we were able, however, to get increased funding from DOE BES.

The principles I used to fund research projects were as follows:

- Pick research at the frontier of science and technology that is applicable to weapons programs.
- Pick projects that have the potential for multiple impacts to multiple customers. Try to foster projects motivated by more than one reason.
- Seek DOE Basic Energy Sciences (BES) (especially Materials Sciences) and MFE (Magnetic Fusion Energy) funding to complement the more targeted weapon's funded research.

It was extremely important to recruit outstanding staff, both to conduct the research and to become future supervisors and managers.

VIII Ion Beam Research

There are several large and focused programs that took considerable investment of people and budgets over many years. One of those programs is the ion beam research area. In Figure 8-1 is a chart of the growth of ion beam research and facilities over the nearly 40 years in my Org. 1100. There was a large increase in the number of accelerators especially in Bldg. 884 where they are still actively used today in the new Ion Beam Laboratory, Bldg. 720. I was particularly fortunate to hire a new staff member, Barney Doyle, to lead the installation and operation of a 6MV Tandem Van de Graaff accelerator. A picture, Figure 8-2, shows, back to front: Barney Doyle, Norman Wing, Paul Peercy, and myself. Barney is today the manager of this operation, which has received five R & D 100 awards for their innovative research. I was fortunate to collaborate with him on several papers.

It is hard to overemphasize the importance of ion beam analysis to Sandia research. Tom Picraux came to my division in 1967 and had expertise in ion beam research. He and I applied these techniques to the analysis of neutron tube films. These allowed the non destructive determination of the depth distribution of elements with a 200 angstrom (about 200 atomic lattice spacings; 1 angstrom = 10^{-8} cm) resolution throughout the first micron of a surface. Using the 2.5 MV Van de Graaff in Bldg. 884 we made the first quantitative depth distribution measurement of the atomic elements in neutron tube films. This was a wonderful discovery to determine directly the depth distribution of the film's elements by Rutherford ion backscattering of deuterium ions. In addition, by using other nuclear reactions we could determine the quantitative depth distribution of hydrogen isotopes. Such measurements are still in use today. Wendland Beezhold used the accelerators to directly measure the operational degradation of the hydrogen isotopes in neutron tube films. Later we used ion backscattering to determine the depth distribution of germanium and silicon in thermoelectric materials for Sandia's Radioisotopic Thermoelectric Generator, RTG.

By combining ion channeling with ion beam analysis, Tom and I could determine the lattice location of hydrogen and helium impurities in single crystal materials such as silicon, tungsten, and chromium. When I gave a talk on these results at Oak Ridge National Laboratory, Don Stevens, director of DOE's Basic Energy Sciences (BES) Material Sciences Division was in the audience and was so impressed with the results that he told me, "We should be funding that work." Up to that time DOE Defense Programs was funding all the basic science work at Sandia. DOE Basic Energy Sciences wanted to be known as funding the best fundamental science in the U.S. As a result of Don Stevens's encouragement we submitted a proposal to BES and became the first program funded by BES at Sandia Albuquerque. This led to other BES funded programs to the point that now BES is the major funding organization for fundamental research at Sandia.

In 1990 George Samara and I wrote a proposal to BES competing for a congressionally authorized $5 million materials science center. Our proposal for a DOE Center of Excellence for the Synthesis and Processing of Advanced Materials won the initial competition for the Center, and Sandia was given the responsibility for coordinating its activities. The Center was established in late FY1991, and George Samara was the Director of this distributed Center until it ceased operation in FY 2005. Working agreements or collaborations were in place with over 50 companies, laboratories, and universities. The technical focus of the Center was in selected areas of atomically structured materials, metals, alloys, polymers, and ceramics.

In recent years BES has funded a new Center for Integrated Nanotechnologies (CINT) which is directed by Sandia and Los Alamos. For his past ion beam research, Tom Picraux received the DOE E.O. Lawrence Award, and Tom is now the Chief Scientist of CINT. CINT is a major new initiative for Sandia fundamental science.

George Samara and I were the managers of the Sandia BES Materials Science Program for many years and paid particular attention to the management of the research to choose, encourage, and insure the highest quality. We were gratified that our program, judged by our peers at other DOE laboratories, received many Outstanding Accomplishment Awards from the Office of Basic Energy Sciences. The proportion of the awards that we received was much larger than the proportional funding of Sandia's BES program. From 1985 through 1993 Sandia received 19 DOE Basic Energy Sciences Outstanding Accomplishment Awards, more than any other Laboratory. From 1987 through 1994 Sandia received 5 BES New Initiative Awards. No other laboratory received more awards.

The use of ion beams to analyze hydrogen isotopes and helium in materials is a very powerful research and application tool. We could now measure hydrogen in fusion reactor wall materials This was very important to the DOE Tokomak magnetic fusion reactor program. As a result we were successful in obtaining new funding from DOE's Magnetic Fusion Energy (MFE) Division. Tokomak magnetic fusion energy reactors require that the plasma (to be heated to fusion temperatures) be magnetically confined away from the walls of the reactor. Plasma physicists, who believed that the wall material should be a high temperature metal such as tungsten to protect the wall after a disruption, previously dominated magnetic fusion research. They did not realize that the plasma is not completely confined away from the wall, and that even a one-micron sphere of a high Z material like tungsten when sputtered off the walls and vaporized will be ionized and completely quench the

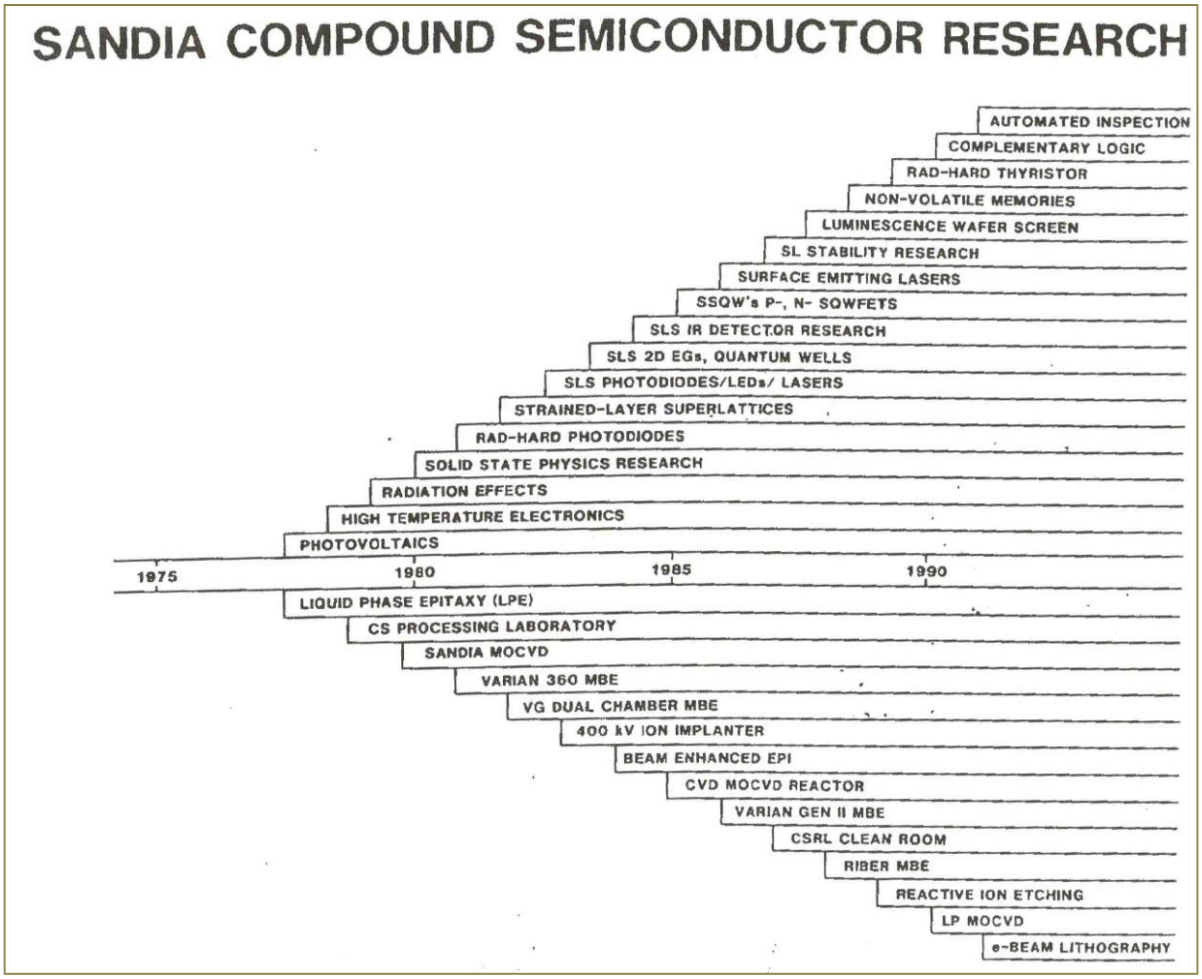

Figure 8-3. Timeline of programs (top) and facilities (bottom) associated with Sandia's compound semiconductor and optoelectronics research.

plasma by emitted x-ray irradiation. Even Japan built their first Tokomak with a complete molybdenum first wall. After a hard learning experience graphite became the preferred first wall material.

In a particular case, research was crucial to determine what would be the retained tritium in the first wall of the TFTR (Tokomak Fusion Test Reactor), the first tritium containing Tokomak reactor, which was being built at Princeton University. Because of tritium's radiation toxicity there was a 5 gm limit of tritium on the Princeton site. It would be catastrophic to the program to have all the tritium reside in the wall and none in the plasma of the reactor. Bill Wampler was funded for many years by MFE's first wall program to assess the inventory of hydrogen isotopes in first wall materials.

Another powerful use of both ion beam analysis and implantation was to study defects in semiconductors. Sam Myers has researched this area in many ways including the determination of the energetics of defect formation and trapping of hydrogen in silicon and in gallium nitride. He also used ion backscattering to study diffusion in materials with extremely high precision to low temperatures. Recently (2006) he is conducting radiation damage research to calculate the damage to silicon devices from a neutron burst from a pulsed reactor such as SPR (Sandia Pulsed Reactor).

IX Compound Semiconductor Research and Strained Layer Superlattices

A second large, focused, and successful program of the 1100 Directorate was development of compound semiconductor and optoelectronics research. George Samara started the effort in the late 1970's by obtaining the first funding from ERDA (the Energy Research and Development Agency- the successor to the Atomic Energy Commission) for work on high temperature electronics, mostly GaP. Defense Program funding for radiation–tolerant III-Vs followed. We built the first radiation–tolerant GaAs photodiode at Sandia. Around 1979 George Samara hired Gordon Osbourn, who started the strained layer

COMPOUND SEMICONDUCTOR LABS AT SANDIA

1978–1979	Began in Isolated Labs in 806 & 807
1980	CSL Located in First Floor 806 with Clean Benches
1981	First MBE
1982	Proposal For New Clean Room CSRL Agreed to at 1000 Level
1983	Decided to Locate CSRL in 893
	Design Consultant Hired in Late 1983
1984	$1.33M GPP and Major Capital were Secured for FY85 Construction
	Plant Engineering Work Request Initiated
1985	Final Layout in January 85
	Request for A&E Design August 85
1986	Early '86 Design Contract Let
	Report of Compound Semiconductor Committee and Plans for Line Item Building
	April CSRL Design Cost Estimate Received
	Plant Eng Estimates; Construction Starts 7/86; Complete 1/8/88
1988	Construction Completed October
1989	Occupancy of CSRL March

Figure 8-4. Key dates and events beginning with the first small isolated compound semiconductor laboratories in 1978 leading to the occupancy of the Compound Semiconductor Research Lab (CSRL) in 1989.

superlattice work around 1980. Later Paul Peercy was the manager of this program for many years.

Compound semiconductors are important for many reasons. For Sandia weapon applications they are of interest to include optics in weapon systems and for microwave devices. In addition, for energy and other applications compound semiconductors are useful for photovoltaics, high temperature electronics, radiation-hard photodiodes, surface emitting lasers, and infrared detectors. The compound semiconductor program required large capital equipment expenditures, and the hiring and organizing of people who had expertise in solid state physics, crystal growth material sciences, and device physics. Figure 8-3 gives the history of the introduction of the necessary equipment and the corresponding indicated research.

There was a ten-year program of systematically growing the capabilities and research base for the compound semiconductor research. A table in Figure 8-4 shows the start of the program in 1978 leading to the occupancy of the Compound Semiconductor Research Lab (CSRL) in 1989. Primarily capital and operating funds from weapons research programs, $10 million from DARPA, and fundamental research funding from DOE BES funded the program. A brand new lab for compound semiconductor research and development was occupied just recently in 2006.

One of the most significant accomplishments of the Organization 1100 compound semiconductor program was the invention and development of Strained Layer Superlattices, or SLS. Strained Layer Superlattices opened up a whole new field (not simply a single new material) of high quality structured semiconductor materials and devices. SLSs use solid state quantum theory in combination with advanced crystal growing techniques to "tailor make" specialized device-quality semiconductors. These take the form of composite sandwich structures of many extremely thin crystalline layers. Because the layer compositions, thickness and numbers may be varied by design over wide limits, the possibility arises of obtaining an infinite number of man-made semiconductor materials.

The concept of multiple semiconductor layers was not new, having been proposed by Esaki nearly 15 years earlier. Early experiments showed (and it was believed until the Sandia work) that the crystalline layers must all have the same atomic lattice constant to within 0.1% to avoid strain induced defects such as dislocations, which ruin the electronic properties. Gordon Osbourn proposed and Organization 1100 showed that high-quality semiconductor superlattices could be made from lattice mismatched semiconductors, and that the strain and orientation, could be tailored to give specific electronic properties.

The first theoretical calculations of the electronic properties of SLSs including the band structure as a function of layer thickness and lattice constant were made by Gordon Osbourn in 1982. Shortly afterward Robert Biefeld grew the first high quality SLSs using metal organic chemical vapor deposition (MOCVD). Luminescence measurements by Paul Gourley confirmed the theoretical predictions. Taken together, the theory, crystal growth, and measurements demonstrated that high quality semiconductor materials could be made from lattice mismatched materials.

Large-scale efforts in 1100 and at other laboratories began to explore various semiconductor systems with differing properties. We were able to show that SLSs could also be made by molecular beam epitaxy (MBE) and that devices with excellent characteristics could be made, and that they could be doped both n and p type. We were also able to show that the electronic properties of devices could be as good as, or even better than, those of bulk or lattice matched materials and that a whole host of new materials could be created atomic layer by atomic layer. For example, luminescence can be made to greatly exceed that obtainable from the bulk materials that make up the layers, despite the many strained interfaces. Subsequent results from many laboratories showed that injection and photo-pumped lasers could be made from them, confirming their high quality electronic and optical properties. Sandia made significant contributions to the development of high quality vertical cavity surface emitting lasers (VCSELS).

X Laser Research

Shortly after I became director of 1100 I inherited a group that was conducting laser research in another organization. This group previously under Jerry Yonas had been pursuing laser initiated inertial confinement fusion. Since Yonas had decided to

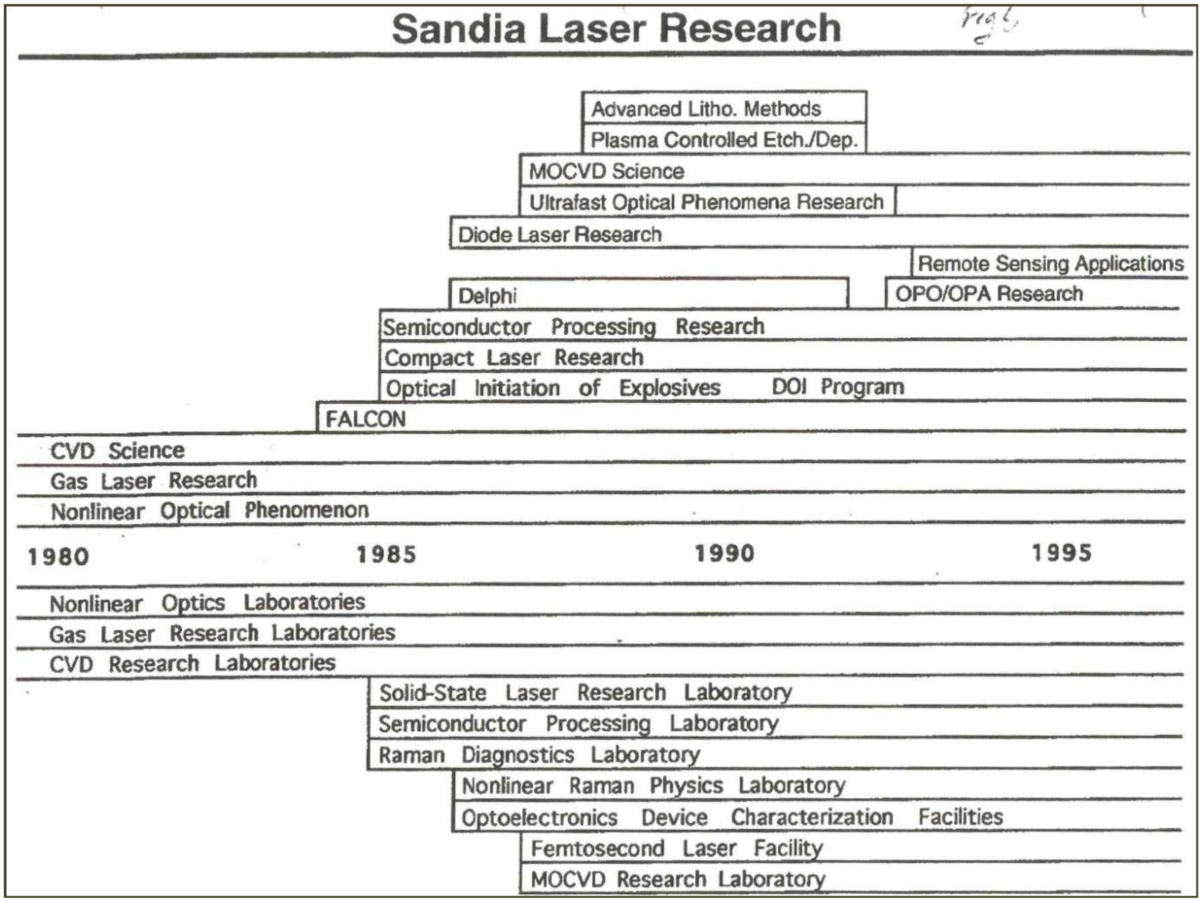

Figure 8-5. Timeline of programs (top) and facilities (bottom) associated with laser research at Sandia (1980-2000).

focus on electron beam fusion (using an electron beam fusion accelerator, EBFA) and then later on ion beam fusion, he was no longer willing to support laser fusion. We needed to find other important scientific research and applications for this group, headed by Jim Gerardo. Figure 8-5 shows the history of the development of laser facilities and programs. Important research accomplishments included the use of lasers to diagnose the physics and chemistry of chemical vapor deposition. A broader application was semiconductor processing research. A successful proposal developed by Gerardo was made to SEMATEC, (the Semiconductor Manufacturing Technology Consortium), of a program to help the U.S. semiconductor equipment industry advance semiconductor processing equipment. This Sandia program was called SETEC for Semiconductor Equipment Technology and received Sandia's first funding from SEMATEC. SETEC became an important new interaction of a National Lab with the U.S. semiconductor industry. In 1987 I gave a talk entitled, " Coupling Sandia's Capabilities to the US. Semiconductor Industry" at a meeting entitled, "DOE National Laboratories and the Semiconductor Industry - Continuing the Joint Planning". The semiconductor industry began to take notice of the capabilities of the National Labs, and subsequently I was asked to summarize the capabilities of all the National Labs at a meeting held by SEMATEC at Monterey, CA.

There were several other strong laser programs under Gerry Hays, who succeeded Jim Gerardo as manager. Laser remote sensing using optical paramagnetic oscillators (OPO) is one program that still exists today and has multiple applications in treaty verification, environmental monitoring, chemical/biological warfare detection, and drug interdiction. Sandia's largest SDI (Strategic Defense Initiative) program was FALCON (Fission Activated Laser Concepts). The laser portion of this program was carried out in 1100. The FALCON program was very much supported by DOE Defense Programs, and consisted of fission fragment pumping of rare gas lasers for power beaming to geostationary satellites, as well as theater missile defense.

XI Diagnostics and Sensors

Many of Organization 1100's accomplishments include the invention of new diagnostic techniques and sensors. The Microsensor Division was first established in 1100. One of the earliest inventions was a quartz piezoelectric sensor that was invented by Errol P. EerNisse. This was a temperature compensated stress gauge for down-hole pressure measurements in oil wells. He also invented a double-ended tuning fork resonator for acceleration measurements. Steve Martin invented a range of surface acoustic wave sensors. Barney Doyle has participated in the invention of many diagnostic techniques including Heavy Ion Backscattering (HIBS), the Ion Beam Electron Microscope, the Ion Beam Photon Microscope, the ion beam induced charge technique (IBIC), the K-Map x-ray crystal perfection technique, and others. He has participated in 5 IR-100 R & D Awards. Jack Houston invented the Interfacial Force Microscope, which is a widely used and extremely useful surface science instrument. Paul Gourley invented the Bio-Cavity Laser Microscope. Phil Hargis and Arlie Smith developed optical paramagnetic oscillator light detection and ranging (LIDAR) remote sensing technology that can identify chemicals in parts per million at a kilometer.

Bob Graham and Mark Anderson together with Francois Bauer of the French /German defense laboratory developed the piezoelectric polymer stress gauge for noninvasive shock wave diagnostics. The polymer gauge (piezoelectric polyvinilidene fluoride, PVDF) has turned out to be very successful, and is widely used for laboratory and full-scale weapons testing. George Samara worked out the physics of why it works to over 100 kbar, way beyond the range of other piezoelectric materials like quartz and lithium niobate. Organization 1100 has always been a leader in developing standards for stress/time measurements made at laboratories worldwide.

XII Surface Physics and Shock Wave Physics

Organization 1100 also had small but highly regarded surface physics and shock wave programs. The Surface Physics group continues to do outstanding research. Terry Michalske received the Dillon glass medal and Peter Feibelman received the Davisson and Germer American Physical Society Prize. In our very small shock wave physics program Bob Graham received the American Physical Society Shock Compression Prize. George Samara was awarded the American Chemical Society Prize for Research Management.

XIII Management

One characteristic of my 36 year career at Sandia in the Research Organization was that I always reported to a Bell Labs supervisor except for a few years when I arrived in 1958 under Dick Claassen and for a short time under Orval Jones when he was Director of 1100. The Bell Labs people were Fridolf Smits, Jim Easley, and Vice Presidents George Dacey, John Galt, Bill Brinkman, Venky Narayanamurti, Paul Fleury. When AT&T terminated its contract to run Sandia, Bert Westwood from Lockheed Martin was the new Vice President of Research. Every time I had a new supervisor from outside Sandia, I had to start over to explain and defend our programs. One upside was that the all the vice presidents had an instinctive support for high quality fundamental research. However, after Bill Brinkman went back to Bell Labs, the Vice-President of Research no longer controlled and allocated the defense programs research budget. There was a continual yearly reduction in 1100's weapon supported research budget. Today (2006) the director of 1100 has a small long term weapons research budget. The department managers and staff members have the responsibility to annually re-negotiate their budgets. A result is rather short term LDRD (Laboratory Directed Research and Development) and project funding. The longest term renewable research funding comes from DOE Basic Energy Sciences including the recent CINT funding. CINT and MESA facilities do provide opportunity for forefront research. However, I believe Org. 1100 needs to continually seek future research funding from BES. As 1100's budget became more fragmented, and as more and more compliance initiatives were introduced, 1100 was fortunate to have Alan Nichelason as its administrative manager.

XIV Conclusion

I can enthusiastically say I enjoyed my career at Sandia immensely. It was the best job I could have imagined. It was particularly a privilege to work with so many talented and friendly people in a common desire to conduct excellent research and help enable Sandia to become a highly respected research laboratory.

In 1958 Sandia had a very small and almost unrecognizable research reputation in solid state science. It was a risky career choice for a new Ph.D. graduate to come to Sandia in 1958. There were no highly recognized senior scientists with whom to work or to be mentored by. However, the managerial guidance of the Bell Labs people, the self-selection of aggressive young scientists and the strong funding (including the DOE Office of Science) enabled the subsequent success. Throughout the period from 1958 through 1994 the reputation of Sandia's Org. 1100 solid state science research stature continually grew, and it became one of the leading research laboratories in the world.

8 Appendix 3. Samuel M. Myers, "Impact of BES research on national security: Fast-transient neutron irradiation of electronics" (February 8, 2011 revision)

Editor's Note: This Appendix contains a short account of Dr. Samuel M. Myers on the impact of research on defects in semiconductors, supported by the Office of Science (Office of Basic Energy Sciences), on our ability to develop methodologies for qualifying devices without the requirement of testing in large-scale neutron sources. As discussed in Section 4.1, such efforts to develop ever-more-accurate predictive understanding of radiation effects have taken on greater urgency with recent decisions to phase out large neutron sources.

Science-Based Stockpile Stewardship at Sandia National Laboratories initiated a new thrust in the Fall of 2004 to deal with the qualification of electronic systems for operation under fast-transient neutron irradiation. The immediate impetus for this effort was the impending shutdown, in September 2005, of the Sandia Pulse Reactor (SPR-III), a fast-burst fission reactor that enabled a key element of experiment-based system evaluation. The new project, entitled "Qualification Alternatives to SPR" (QASPR), is combining experiments in available irradiation facilities, mechanistic simulations of time-dependent damage effects in devices and circuits, and supporting theoretical and experimental studies in order to develop protocols for robust prediction of system behavior. Of greatest present interest are bipolar transistors based on Si and on III-V heterostructures, with emphasis on the latter increasing during 2010. Actual QASPR involvement in system design and engineering is intended to begin in 2012 and grow through the remainder of the decade. Major demonstration milestones have already been met for the simulation of Si-based devices and circuits, with prototype demonstrations for the III-Vs to begin in 2011. The QASPR project involves multiple organizations within Sandia and is managed by Leonard Lorence of the Radiation Sciences Center.

Sandia's Center for Physical, Chemical, and Nano Sciences has principal responsibility for two central elements of QASPR.

The first responsibility is the identification, understanding, and quantitative mechanistic description of relevant physical processes involving the formation, transport, and reactions of irradiation defects and carriers in bipolar devices, with ab-initio theory and experiments being carried out to address gaps in existing knowledge.

The second responsibility is to establish pulsed ion-beam irradiation as a quantitative tool for assessing fast-transient neutron effects in Si and III-V devices, with mechanistic understanding serving to optimize the ion-beam treatments and account for differences between ion and neutron damage. Progress in these two areas of QASPR has been made possible by prior advances associated with BES programs in the Center; without this enabling basis, progress would have been far slower and probably inadequate for the upcoming schedule of systems development. In the following, four specific areas of BES impact are discussed.

Density-functional theory of defects in semiconductors

Density-functional theory (DFT) is presently the best widely applicable tool with which to calculate the formation energies, and thereby the relative stabilities, of defect configurations in their various charge states within semiconductors. In support of atomistic modeling in the QASPR project, DFT is used to obtain bandgap electronic levels for relevant defects; paths and associated activation barriers for diffusion; and binding energies for the primal defects with dopants, impurities, and other defects. The challenge of DFT is that its accuracy for semiconductors is now only ~ 0.1 – 0.2 eV, and even that is strongly dependent on the details of the calculations in ways that are incompletely understood. Prior BES studies of defects and hydrogen in Si and GaN served to establish optimum methodologies and contributed to the development of an in-house code (Socorro) combining the necessary capabilities with efficient massively parallel execution.

Figure 9-1 exemplifies DFT capabilities established under BES and exploited in the QASPR effort. The sequence of configurations for H in GaN, taken from BES work reported in 2003, shows the predicted diffusion path responsible for H migration along the c-axis of the hexagonal lattice in p-type material.[63] A key aspect of this result is the activation energy for the diffusion process, equal to the energy

[63] AF Wright, CH Seager, SM Myers, DD Koleske, and AA Allerman, J. Appl. Phys. **94**, 2311 (2003).

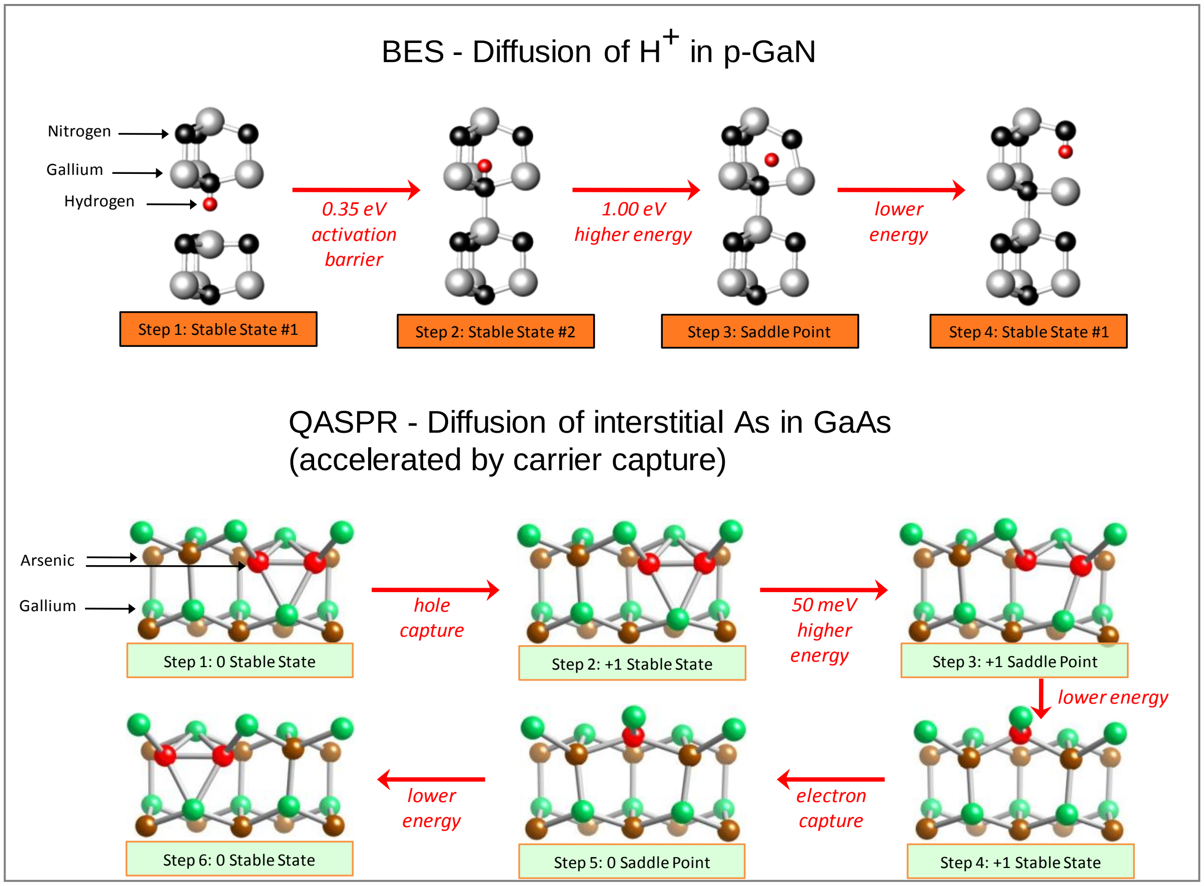

Figure 9-1. Top: Sequence of configurations for diffusion of H along the c-axis of the hexagonal lattice in p-type GaN. Bottom: Sequence of configurations for migration of interstitial As in GaAs via the combined effects of thermally activated atomic motion and configurational changes associated with successive capture of holes and conduction electrons.

difference of 1.0 eV between the stable states and the saddle point.

The lower configuration sequence for interstitial As in GaAs, from QASPR work in 2010, shows the use of newly refined DFT methods to treat a more complex problem: migration of the interstitial defect via the combined effects of thermally activated atomic motion and configurational changes associated with successive captures of holes and conduction electrons. [64] The resulting diffusion depends relatively weakly on temperature but is strongly influenced by carrier-injection effects in electronic devices.

Minimizing and knowing the uncertainties of DFT predictions is exceptionally important to QASPR, and the resulting attention given to this aspect of the theory has yielded advances with wide implications. One example is the influence of interactions among the repeating lattice cells used to treat point defects within crystalline semiconductors, particularly defects in high charge states. QASPR studies have shown that the combination of long-range electrostatic and strain fields can produce errors as large as several tenths of an eV for cell sizes typically used in the theoretical community. This source of error can be largely removed by calculations at several cell sizes, ranging up to the large dimensions now made possible by massively parallel computing, followed by physics-based extrapolation to infinity.[65]

Mechanistic description of the intertwined behaviors of defects and carriers

Sandia's BES studies of hydrogen and defects in GaN advanced from the above theoretical predictions of atomic configurations and energetics to a quantitative consideration of implications for thermodynamics and the kinetics of migration and reactions among the various species under the influence of internal fields. This led in turn to model codes simulating the global behavior of device

[64] AF Wright, to be published.

[65] AF Wright, Phys. Rev. 74, 165116 (2006).

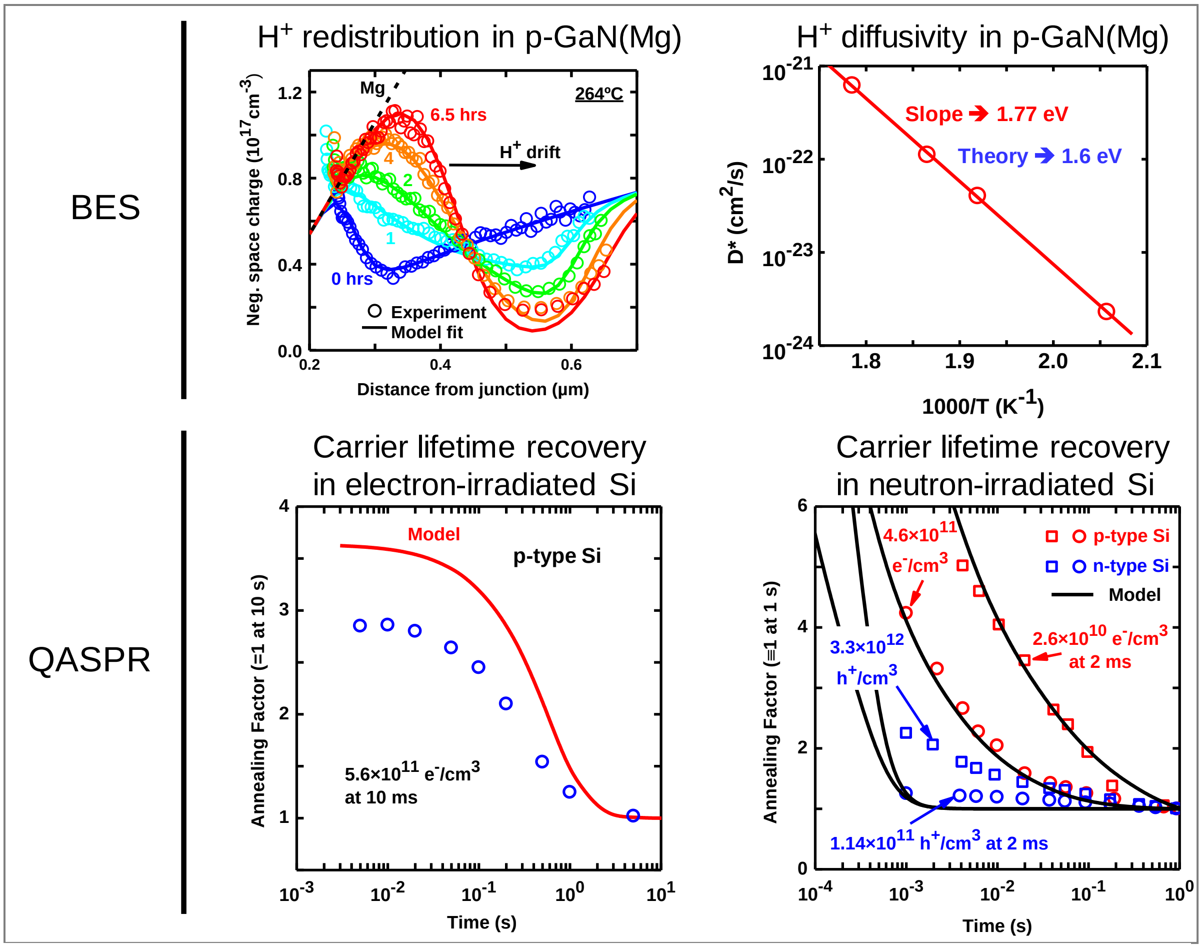

Figure 9-2. Mechanistic simulations of the transient behavior of impurities, defects and carriers, initially in the BES program in 2003 (above), and later under the QASPR program in 2008 (below). As discussed in more detail in the text, the upper panel shows (left) the evolution of net space charge during annealing of a reverse-biased pn junction at a particular temperature, and (right) the inferred effective H diffusion coefficient, D*, at a number of temperatures. Also as discussed in more detail in the text, the lower panel shows the evolution of the annealing factor (a measure of the recovery of minority-carrier lifetime during annealing of damage after pulsed irradiation with electrons or neutrons) in the much more complex problem of transient irradiation effects in working semiconducting devices.

structures. These capabilities translated directly into QASPR modeling, so that within a year of the advent of the latter project, a first-version simulation of a Si bipolar transistor provided a seamless description of carriers and an array of irradiation defects migrating and undergoing reactions. This immediately accounted in first order for the observed transient behaviors of neutron-irradiated devices, providing an advanced point of departure for the refinements that have followed.

Figure 9-2 shows mechanistic simulations of the transient behavior of impurities, defects and carriers, initially in the BES program in 2003, and later under QASPR in 2008. The first of the upper panels exhibits the redistribution of H+ in the p-type region of an n+/p diode that was first equilibrated under zero bias and then maintained under a reverse bias of 12 V at a temperature of 264ºC for times from zero to 6.5 hrs.[66] The plotted quantity is net space charge versus distance into the p-region from the junction, as measured by C-V methods and simulated by a theoretical model of the device; the observed evolution arises from the movement of the positive H from left to right under the influence of the bias-induced internal field. The effective H diffusion coefficient, D*, obtained by fitting of the theoretical model to C-V data, is shown as a function of temperature in the Arrhenius plot at upper right. The activation energy of 1.77 eV is in satisfactory agreement with the sum of the DFT-predicted diffusion barrier reported in Figure 9-1, 1.0 eV, and

[66] AF Wright, CH Seager, SM Myers, DD Koleske, and AA Allerman, J. Appl. Phys. **94**, 2311 (2003).

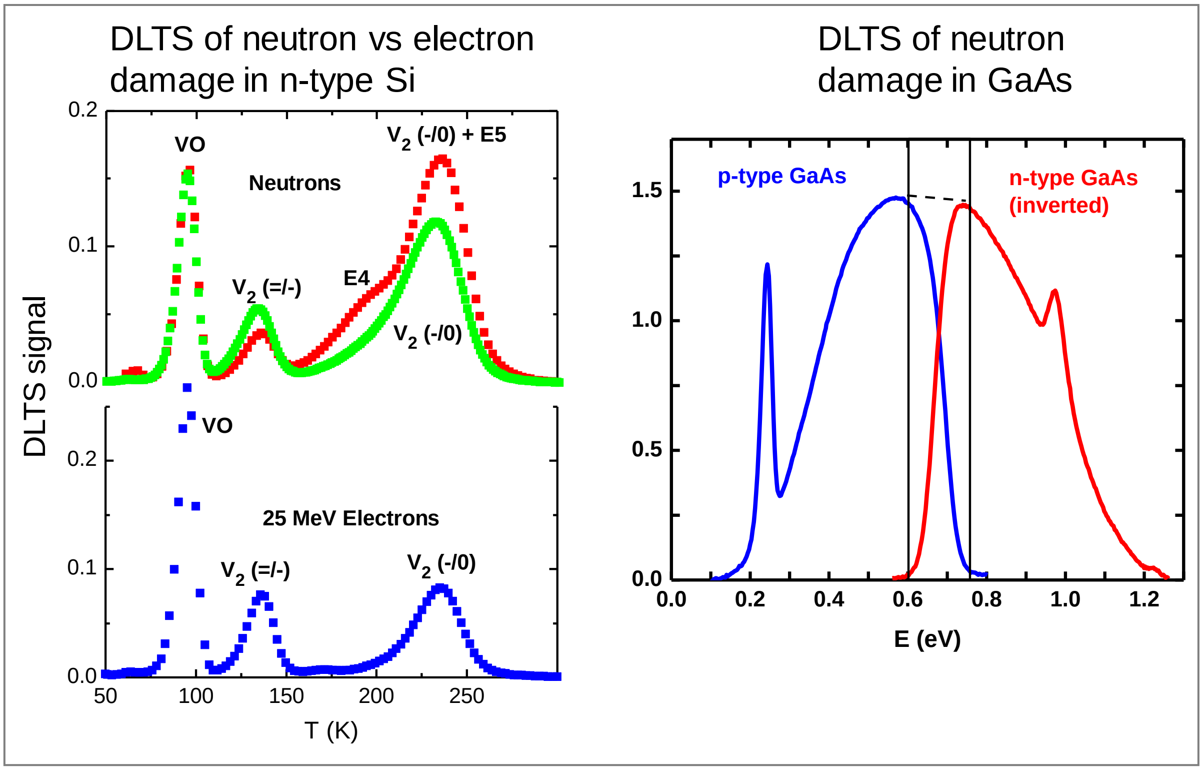

Figure 8-3. Deep level transient spectroscopy (DLTS) data, in order of increasing complexity, as discussed in the text, for electron (left bottom) and neutron (left top) displacement damage in Si, and neutron displacement damage in GaAs.

the binding energy predicted for transient trapping of H+ at Mg dopants, 0.6 eV.

In the QASPR project, the same basic approach to modeling of the transport and reactions of charged mobile species in semiconductors was extended to the much more complex problem of transient irradiation effects in semiconducting devices. The lower panels in Figure 9-2 show the recovery of minority-carrier lifetime in uniform bulk Si due to the thermally activated evolution of damaged after pulsed irradiation with electrons or neutrons. [67] Minority carriers were injected at various fixed rates during several damage-evolution sequences, leading to minority-carrier concentrations that rose with the increasing lifetimes and reached the indicated levels at 2 or 10 ms. The plotted Annealing Factor is related to carrier lifetime, τ, by

$$AnnealingFactor = \frac{\tau^{-1}(t) - \tau^{-1}(prerad)}{\tau^{-1}(t = t_1) - \tau^{-1}(prerad)},$$

where t_1 is 2 or 10 ms. The simulation results in the plots arise from seamless modeling of the diffusion, field-drift, and reactions of conduction electrons, holes, and 35 primal and secondary defect species in their multiple charge states; these simulations are predictive rather than fitted. Of particular note are the large, qualitative differences between MeV electron irradiation, where the primal vacancies and interstitials are randomly dispersed, and neutron irradiation, where the defects are localized in recoil cascades.

Defect characterization by deep-level transient spectroscopy

Deep-level transient spectroscopy (DLTS) and related techniques are the principal means for identification of irradiation defects within devices in the QASPR project. Expertise and experimental facilities were developed and refined during decades of BES research for the case of isolated point defects in simple diode structures. In the context of QASPR, these capabilities have been fundamentally extended to encompass defects formed within the dense recoil cascades of neutrons, and further to allow analyses of bipolar transistors. This has permitted validation of atomistic models and sensitive assessment of the degree of similarity between neutron damage and the ion damage used to simulate it.

Figure 9-3 shows DLTS data illustrating the leaps in complexity of irradiation displacement damage encountered in the QASPR project upon going from electron-produced point defects to the neutron damage

[67] SM Myers, PJ Cooper, and WR Wampler, J. Appl. Phys. 104,044507 (2006).

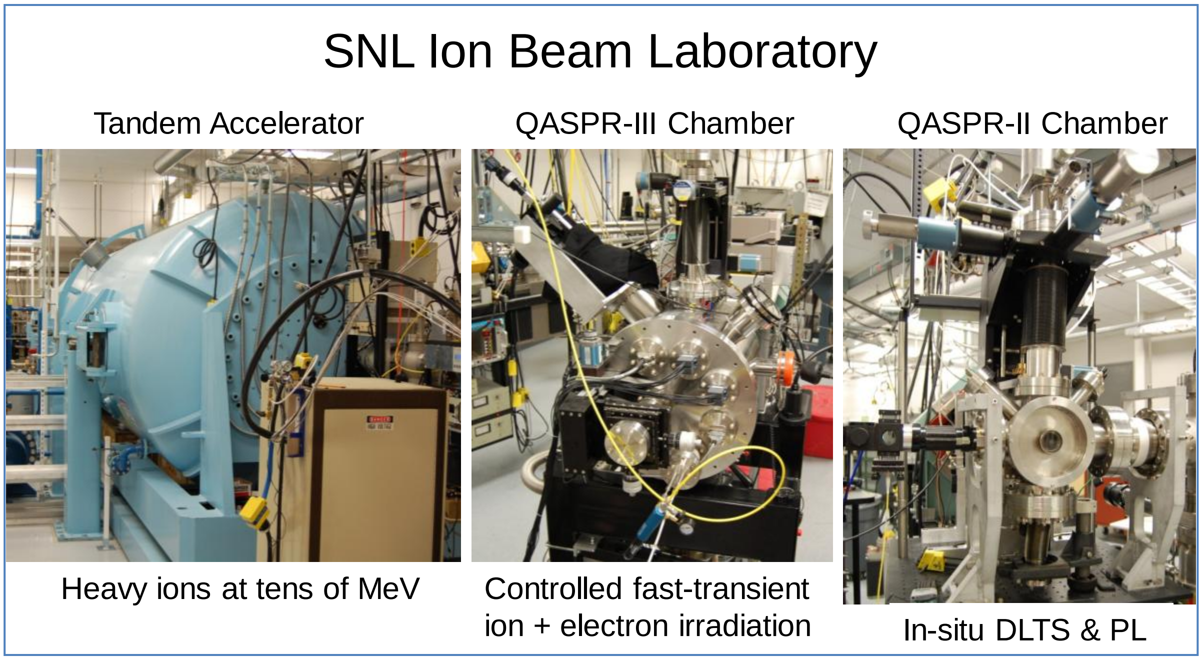

Figure 9-4. The 6-MV tandem ion accelerator, along with two target chambers that were developed under the QASPR project to allow mechanistic studies of transient irradiation effects in semiconductor devices.

that is of primary interest.[68] In the case of Si, the lower plot in the left-hand panel exhibits the familiar DLTS peaks that result from electron irradiation of n-type material followed by thermally activated diffusion and reaction of the primal defects at room temperature; the spectrum is dominated by the signature of the isolated vacancy-oxygen complex along with two electronic transitions of the isolated divacancy. In the contrasting spectra from neutron-irradiated Si, the second of the two divacancy peaks is substantially larger than the first, an effect provisionally ascribed to field-induced band-bending and possibly strain-mediated defect-defect reactions within the high-density core of the recoil cascade. Moreover, there is also a bistable defect, believed to be of vacancy type, that reversibly exhibits and loses peaks E4 and E5 during successive treatments of current injection and open-circuit annealing. (The latter effect, prominent in neutron-irradiated material, has recently been detected in electron-irradiated Si as well.)

The complexity of neutron damage is still greater in GaAs, where the recoil cascades are more dense than in Si and there is less thermally activated evolution at room temperature. The right-hand graph in Figure 9-3 superimposes DLTS spectra from p- and n-type material, with the latter inverted on the horizontal axis and temperature converted to energy level in the bandgap. The very broad band of transition energies reflects a wide range of electronic transition energies within the dense core of the recoil cascades, presumably reflecting a combination of damage complexity and the influence of very large local electrostatic fields. (The cutoffs at midband are an inherent artifact of the DLTS measurement.) The two sharp peaks, which grow at room temperature after the irradiation pulse, are inferred to arise from reacted defect complexes outside the cascade core, probably involving the dopants.

Ion-solid interactions and ion damage in semiconductors

In 1977 Sandia began the BES program "Ion Implantation and Defects in Materials," later renamed "Energetic-Particle Synthesis and Science of Materials," which continues to the present. Spanning a range of phenomena in semiconductors, insulators, and metals, this effort yielded broad experimental expertise and a widely ranging, in-depth understanding of ion-solid interactions. Combined with the continuously advancing facilities of Sandia's Ion Beam Laboratory, notably including a tandem accelerator that provides heavy-ion beams at tens of MeV, this enabled project-critical ion irradiations of devices from the early stages of QASPR.

Figure 9-4 shows the 6-MV tandem ion accelerator, along with two target chambers that were developed under the QASPR project to allow mechanistic studies of transient irradiation effects in

[68] RM Fleming, CH Seager, DV Lang, E Bielejec and JM Campbell, J. Appl. Phys. 104 (8), 083702-083710 (2008); and RM Fleming, DV Lang, CH Seager, E Bielejec, GA Patrizi and JM Campbell, J. Appl. Phys. 107 (12), 123710-123715 (2010).

semiconductor devices. QASPR-III provides concurrent displacement damage through ion bombardment and ionization with an electron beam, enabling the characterization of transient synergistic phenomena. QASPR-II allows in-situ DLTS of defects and photoluminescence detection to measure time-dependent carrier lifetimes. These extended capabilities now provide an enhanced capability for fundamental studies of radiation effects at Sandia.

Concluding remarks

The interrelationship between BES-sponsored research on defects and atomic processes in semiconductors and the mission-oriented QASPR project has contributed importantly to both efforts, in areas extending from ab-initio theory to modeling of atomic processes and to experiment. The examples given above exemplify this mutually beneficial synergy, which may suggest parallels in other activities of the Laboratories.

9 Appendix 4: Sandia National Laboratories articles with ≥ 200 cumulative citations, Sorted by Citation Count

Front Bracket:

Number of citations in the Institute of Scientific Information's web of science database as of December 2010.

End Bracket:

Funding Source.

Funding Source Abbreviations:

DOE-NW/NA: Funding through the Department of Energy, either through a Nuclear Weapons Office or without further attribution within the Department of Energy.

DOE-SC: Funding through the Department of Energy, Office of Science.

DOE-Non-SC/non-NW: Funding through any Department of Energy office other than a Nuclear Weapons Office or the Office of Science.

NSF/NIH: Funding through the National Science Foundation or the National Institute of Health.

LDRD: Funding through the Sandia Laboratory Directed Research and Development Program.

DoD: Funding through the Department of Defense.

Other: Funding through any other source not previously listed.

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10 Appendix 5: Sandia National Laboratories articles with ≥ 100 cumulative citations, Sorted by Author Name

First Bracket:

Number of citations in the Institute of Scientific Information's web of science database as of December 2010.

Second Bracket:

Funding Source.

Funding Source Abbreviations:

DOE-NW/NA: Funding through the Department of Energy, either through a Nuclear Weapons Office or without further attribution within the Department of Energy.

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Other: Funding through any other source not previously listed.

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